Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

Exercises on Quantum Mechanics II (TM1/TV)

Problem set 8, discussed December 9 - December 13, 2019

Exercise 48

Consider the motion of a particle in a potential $V(q(t))$. Show that the second order of the perturbation expansion of the propagator $K(f,i) = K(q_f, q_i; t_f, t_i)$ can be written as

$$K^{(2)}(f,i) = -\frac{1}{\hbar^2}\int_{t_i}^{t_f} \mathrm{d}t_{II} \int_{t_i}^{t_{II}} \mathrm{d}t_I \int\limits_{-\infty}^{+\infty} \mathrm{d}q_{II} \int\limits_{-\infty}^{+\infty} \mathrm{d}q_I K^{(0)}(f,II)V(II)K^{(0)}(II,I)V(I)K^{(0)}(I,i)$$

Here II and I represent (q_{II}, t_{II}) and (q_I, t_I) respectively and $t_{II} > t_I$.

Solution:

The exact propagator is given by:

$$K(q_f, q_i; t_f, t_i) = \int\limits_{\left\{\substack{q(t_f)=q_f \\ q(t_i)=q_i}\right.} \mathscr{D}q \exp\left\{\frac{i}{\hbar}(S_0 - \int_{t_i}^{t_f} V(q(t))\mathrm{d}t)\right\}$$

The exponential in the integral can be expanded in terms of the potential and therefore also $K(f,i)$ can be expanded:

$$\exp\left\{\frac{i}{\hbar}(S_0 - \int_{t_i}^{t_f} V(q(t))\mathrm{d}t)\right\} = \exp\left\{\frac{i}{\hbar}S_0\right\}\left(1 - \frac{i}{\hbar}\int_{t_i}^{t_f} V(q(t))\mathrm{d}t - \frac{1}{2\hbar^2}\int_{t_i}^{t_f} V(q(t))\mathrm{d}t \int_{t_i}^{t_f} V(q(t'))\mathrm{d}t'\right)$$

$$\Rightarrow K^{(0)}(f,i) = \int\limits_{\left\{\substack{q(t_f)=q_f \\ q(t_i)=q_i}\right.} \mathscr{D}q \exp\left\{\frac{i}{\hbar}S_0\right\}$$

$$K^{(1)}(f,i) = -\frac{i}{\hbar}\int\limits_{\left\{\substack{q(t_f)=q_f \\ q(t_i)=q_i}\right.} \mathscr{D}q \exp\left\{\frac{i}{\hbar}S_0\right\}\int_{t_i}^{t_f} V(q(t))\mathrm{d}t$$

$$K^{(2)}(f,i) = -\frac{1}{2\hbar^2}\int\limits_{\left\{\substack{q(t_f)=q_f \\ q(t_i)=q_i}\right.} \mathscr{D}q \exp\left\{\frac{i}{\hbar}S_0\right\}\int_{t_i}^{t_f} V(q(t_{II}))\mathrm{d}t_{II}\int_{t_i}^{t_f} V(q(t_I))\mathrm{d}t_I$$

We can interchange the integration variables and use the fact that we can split the path integral in the following way:

$$\int\limits_{\left\{\substack{q_f \\ q_i}\right.} \mathscr{D}q \mathrm{e}^{\frac{i}{\hbar}S_0} = \int\limits_{-\infty}^{+\infty} \mathrm{d}u \int\limits_{\left\{\substack{q_f \\ u}\right.} \mathscr{D}q \mathrm{e}^{\frac{i}{\hbar}S_0} \int\limits_{\left\{\substack{u \\ q_i}\right.} \mathscr{D}q \mathrm{e}^{\frac{i}{\hbar}S_0}$$

Then the first order propagator is given by:

$$
\begin{aligned}
K^{(1)}(f,i) &= -\frac{i}{\hbar}\int_{t_i}^{t_f}\mathrm{d}t_I \int\limits_{-\infty}^{+\infty}\mathrm{d}q_I \int\limits_{\substack{q(t_f)=q_f\\ q(t_I)=q_I}} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0}V(q_I) \int\limits_{\substack{q(t_I)=q_I\\ q(t_i)=q_i}} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0} \\
&= -\frac{i}{\hbar}\int_{t_i}^{t_f}\mathrm{d}t_I \int\limits_{-\infty}^{+\infty}\mathrm{d}q_I K^{(0)}(q_f,q_I;t_f,t_I)V(q_I)K^{(0)}(q_I,q_i;t_I,t_i)
\end{aligned}
$$

For the second order perturbation we can split the double integral over t_I and t_{II} into the parts where $t_{II} > t_I$ and $t_I > t_{II}$:

$$
\begin{aligned}
\int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_i}^{t_f}\mathrm{d}t_I V(q(t))V(q(t')) &= \int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_i}^{t_{II}}\mathrm{d}t_I V(q(t_I))V(q(t_{II})) + \int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_{II}}^{t_f}\mathrm{d}t_I V(q(t_I))V(q(t_{II})) \\
&= \int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_i}^{t_{II}}\mathrm{d}t_I V(q(t_I))V(q(t_{II})) - \int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_f}^{t_{II}}\mathrm{d}t_I V(q(t_I))V(q(t_{II})) \\
&= 2\int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_i}^{t_{II}}\mathrm{d}t_I V(q(t_I))V(q(t_{II}))
\end{aligned}
$$

where in the last step we have simply used the fact that we can change t_f to t_i in the t_I integral in the second term by just switching the sign in front of it. Now we can also split the path integral:

$$
\int\limits_{\left\{\substack{q_f\\ q_i}\right.} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0} = \int\limits_{-\infty}^{+\infty}\mathrm{d}q_{II}\mathrm{d}q_I \int\limits_{\left\{\substack{q_f\\ q_{II}}\right.} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0} \int\limits_{\left\{\substack{q_{II}\\ q_I}\right.} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0} \int\limits_{\left\{\substack{q_I\\ q_i}\right.} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0}
$$

Plugging these two identites into the equation for the second order perturbation and interchanging the integration variables we get:

$$
\begin{aligned}
K^{(2)}(f,i) &= -\frac{1}{\hbar^2}\int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_i}^{t_{II}}\mathrm{d}t_I \int\limits_{-\infty}^{+\infty}\mathrm{d}q_{II}\mathrm{d}q_I \int\limits_{\substack{q(t_f)=q_f\\ q(t_{II})=q_{II}}} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0}V(q_{II}) \int\limits_{\substack{q(t_{II})=q_{II}\\ q(t_I)=q_I}} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0}V(q_I) \int\limits_{\substack{q(t_I)=q_I\\ q(t_i)=q_i}} \mathscr{D}q\mathrm{e}^{\frac{i}{\hbar}S_0} \\
&= -\frac{1}{\hbar^2}\int_{t_i}^{t_f}\mathrm{d}t_{II}\int_{t_i}^{t_{II}}\mathrm{d}t_I \int\limits_{-\infty}^{+\infty}\mathrm{d}q_{II}\int\limits_{-\infty}^{+\infty}\mathrm{d}q_I K^{(0)}(q_f,q_{II};t_f,t_{II})V(q_{II})K^{(0)}(q_{II},q_I;t_{II},t_I)V(q_I)K^{(0)}(q_I,q_i;t_I,t_i)
\end{aligned}
$$

Exercise 49 (central tutorial)

For solving problems in perturbation theory and initial value problems the Green's function plays an important role. It is defined as the solution to the equation

$$
\hat{H}_x G(\underline{x},\underline{y}) = \delta(\underline{x}-\underline{y}) \tag{1}
$$

where $\hat{H}_x$ is a linear operator acting on x. We want to calculate the Green's function of a massive particle.

(i) The Hamiltonian of the free particle is given by $\hat{H}_0 = \frac{\hat{p}^2}{2m}$. Choose $z \in \mathbb{C}$ such that $\hat{H}_0 - z$ has an inverse defined as $\left\langle \underline{x} \middle| (\hat{H}_0 - z)(\hat{H}_0 - z)^{-1} \middle| \underline{x}' \right\rangle = \delta(\underline{x}-\underline{x}')$. Prove that $(\hat{H}_0 - z)^{-1}$ satisfying

$$
\left\langle \underline{p} \middle| \frac{1}{\hat{H}_0 - z} \middle| \underline{p}' \right\rangle = \delta(\underline{p}-\underline{p}')\left(\frac{\underline{p}'^2}{2m} - z\right)^{-1} \tag{2}
$$

is the inverse of $\hat{H}_0 - z$.
(Use that $\langle \underline{x} \,|\, \underline{p} \rangle = (2\pi\hbar)^{-d/2}\mathrm{e}^{\frac{i}{\hbar}\underline{p}\underline{x}}$, where d is the dimension of $\underline{x}$ and $\underline{p}$.)

(ii) $(\hat{H}_0 - z)^{-1}$ is called the *resolvent* of $\hat{H}_0$. Show that for $d = 3$ one has

$$
\left\langle \underline{x} \middle| \frac{1}{\hat{H}_0 - z} \middle| \underline{x}' \right\rangle = \frac{m}{2\pi\hbar^2\,|\underline{x}'-\underline{x}|}\exp\left(\frac{i}{\hbar}\sqrt{2mz}\,|\underline{x}'-\underline{x}|\right) \tag{3}
$$

(iii) For which values of m and z is (3) a Green's function of the linear operator $-\Delta + k^2$.

(iv) By taking the limit $z \to 0$ we get a Green's function for $\hat{H}_0$. However in certain cases one encounters singularies when taking this limit. One example is the one dimensional resolvent of $\hat{H}_0$. Derive the analogue of (3) for $d = 1$.

(v) By taking the limit $z \to 0$ a singularity arises. In order to avoid that define:

$$G(x, y) = \lim_{z \to 0} \left[\left\langle \underline{x} \middle| \frac{1}{\hat{H}_0 - z} \middle| \underline{x}' \right\rangle - \sum_{i=-\infty}^{+\infty} A_i(x, y)(\sqrt{z})^i \right] \tag{4}$$

Which conditions do the coefficients $A_i(x, y)$ have to fulfill such that $G(x, y)$ converges and is a Green's function of $\hat{H}_0$?

(vi) Consider the one dimensional electrostatic problem

$$\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} = f(x)$$
$$\phi(x) = 0 \text{ for } x \to -\infty \tag{5}$$

where $f(x)$ has compact support on $[0, L]$. Derive an integral expression for $\phi(x)$ which solves (5). Show that the boundary condition in (5) fixes the remaining free parameter A_0. What is the physical interpretation of this model?

Solution:

(i)

$$\begin{aligned}
\left\langle \underline{x} \middle| (\hat{H}_0 - z)(\hat{H}_0 - z)^{-1} \middle| \underline{x}' \right\rangle &= \iint \mathrm{d}^d p \mathrm{d}^d p' \left\langle \underline{x} \middle| (\hat{H}_0 - z) \middle| \underline{p} \right\rangle \left\langle \underline{p} \middle| (\hat{H}_0 - z)^{-1} \middle| \underline{p}' \right\rangle \left\langle \underline{p}' \middle| \underline{x}' \right\rangle \\
&= \iint \mathrm{d}^d p \mathrm{d}^d p' \left\langle \underline{x} \middle| \underline{p} \right\rangle \left\langle \underline{p}' \middle| \underline{x}' \right\rangle \left(\frac{\underline{p}^2}{2m} - z \right) \left\langle \underline{p} \middle| (\hat{H}_0 - z)^{-1} \middle| \underline{p}' \right\rangle \\
&= \iint \frac{\mathrm{d}^d p \mathrm{d}^d p'}{(2\pi\hbar)^d} \mathrm{e}^{\frac{i}{\hbar}\underline{x}\underline{p}} \mathrm{e}^{-\frac{i}{\hbar}\underline{p}'\underline{x}'} \left(\frac{\underline{p}^2}{2m} - z \right) \left(\frac{\underline{p}^2}{2m} - z \right)^{-1} \delta(\underline{p} - \underline{p}') \\
&= \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^d} \mathrm{e}^{\frac{i}{\hbar}\underline{p}(\underline{x} - \underline{x}')} = \delta(\underline{x} - \underline{x}')
\end{aligned}$$

(ii)

$$\begin{aligned}
\left\langle \underline{x} \middle| (\hat{H}_0 - z)^{-1} \middle| \underline{x}' \right\rangle &= \iint \mathrm{d}^3 p \mathrm{d}^3 p' \left\langle \underline{x} \middle| \underline{p} \right\rangle \left\langle \underline{p} \middle| (\hat{H}_0 - z)^{-1} \middle| \underline{p}' \right\rangle \left\langle \underline{p}' \middle| \underline{x}' \right\rangle \\
&= \iint \frac{\mathrm{d}^3 p \mathrm{d}^3 p'}{(2\pi\hbar)^3} \mathrm{e}^{\frac{i}{\hbar}\underline{x}\underline{p}} \mathrm{e}^{-\frac{i}{\hbar}\underline{x}'\underline{p}'} \frac{\delta(\underline{p} - \underline{p}')}{\frac{\underline{p}'^2}{2m} - z} = \int \frac{\mathrm{d}^3 p}{(2\pi\hbar)^3} \frac{\mathrm{e}^{\frac{i}{\hbar}\underline{p}(\underline{x} - \underline{x}')}}{\frac{\underline{p}^2}{2m} - z} \\
&= \frac{1}{(2\pi)^2\hbar^3} \int_0^\infty \mathrm{d}p \int_0^\pi \mathrm{d}\theta p^2 \sin\theta \frac{\mathrm{e}^{\frac{i}{\hbar}p|\underline{x} - \underline{x}'|\cos\theta}}{\frac{p^2}{2m} - z}
\end{aligned}$$

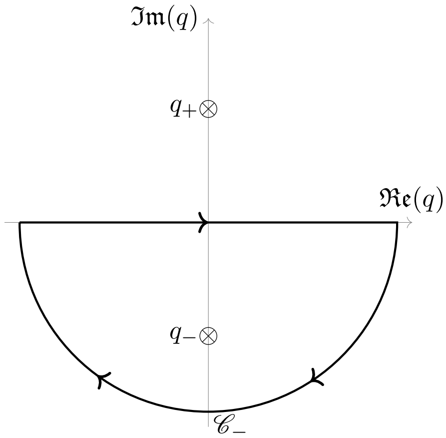
Now we can make the substitution $u(\theta) = \cos\theta$ which leads to $\mathrm{d}u = -\sin\theta \mathrm{d}\theta$ and $u(0) = 1, u(\pi) = -1$. Then the integral becomes:

$$\frac{1}{(2\pi)^2\hbar^3} \int_0^\infty \mathrm{d}p \int_{-1}^1 \mathrm{d}u p^2 \frac{\mathrm{e}^{\frac{i}{\hbar}p|\underline{x} - \underline{x}'|u}}{\frac{p^2}{2m} - z} = \frac{1}{(2\pi)^2\hbar^3} \int_0^\infty \mathrm{d}p \frac{2p}{\frac{p^2}{2m} - z} \frac{\hbar \sin\left(\frac{p}{\hbar}|\underline{x} - \underline{x}'|\right)}{|\underline{x} - \underline{x}'|}$$

To further simplify the notation we rename the follwoing quantities: $q = \frac{p}{\hbar}|\underline{x} - \underline{x}'|$, $\alpha = \frac{\hbar^2}{2m|\underline{x} - \underline{x}|^2}$. So the integral can be rewritten as:

$$\begin{aligned}
&\frac{2}{(2\pi)^2|\underline{x} - \underline{x}'|^3} \int_0^\infty \mathrm{d}q \frac{q \sin q}{\alpha q^2 - z} = \frac{2}{(2\pi)^2|\underline{x} - \underline{x}'|^3} \frac{1}{2i} \left(\int_0^\infty \mathrm{d}q \frac{q\mathrm{e}^{iq}}{\alpha q^2 - z} + \int_0^\infty \mathrm{d}q \frac{(-q)\mathrm{e}^{-iq}}{\alpha q^2 - z} \right) \\
&= \frac{-i}{(2\pi)^2|\underline{x} - \underline{x}'|^3} \left(\int_{-\infty}^0 \mathrm{d}q \frac{(-q)\mathrm{e}^{-iq}}{\alpha q^2 - z} + \int_0^\infty \mathrm{d}q \frac{(-q)\mathrm{e}^{-iq}}{\alpha q^2 - z} \right) = \frac{i}{(2\pi)^2|\underline{x} - \underline{x}'|^3} \int_{-\infty}^{+\infty} \mathrm{d}q \frac{q\mathrm{e}^{-iq}}{\alpha q^2 - z} \\
&= \frac{i}{(2\pi)^2|\underline{x} - \underline{x}'|^3 \alpha} \int_{-\infty}^{+\infty} \mathrm{d}q \frac{q\mathrm{e}^{-iq}}{(q + \sqrt{z/\alpha})(q - \sqrt{z/\alpha})}
\end{aligned}$$

To evaluate this integral we close the integration contour in the lower half of the complex plane at infinity such that the exponential factor in the integral vanishes $\lim_{q\to -i\infty} \mathrm{e}^{-iq} = 0$. As becomes clear from the form of the integral it has two poles at $q_\pm = \pm\sqrt{\frac{z}{\alpha}}$. If z has non-vanishing imaginary part q_- lies within the contour of integration and we can use the residue theorem to evaluate the integral.



$$\frac{i}{(2\pi)^2\,|\underline{x}-\underline{x}'|^3\,\alpha}\oint_{\mathscr{C}_-}\mathrm{d}q\frac{q\mathrm{e}^{-iq}}{(q+\sqrt{z/\alpha})(q-\sqrt{z/\alpha})} = \frac{2im}{(2\pi)^2\hbar^2\,|\underline{x}-\underline{x}'|}(-2\pi i)\mathrm{Res}_{q=-\sqrt{z/\alpha}}\left\{\frac{q\mathrm{e}^{-iq}}{(q+\sqrt{z/\alpha})(q-\sqrt{z/\alpha})}\right\}$$

$$= \frac{m}{\pi\hbar^2\,|\underline{x}-\underline{x}'|}\lim_{q\to-\sqrt{z/\alpha}}\left(\frac{q\mathrm{e}^{-iq}}{(q+\sqrt{z/\alpha})(q-\sqrt{z/\alpha})}(q+\sqrt{z/\alpha})\right) = \frac{m}{2\pi\hbar^2\,|\underline{x}-\underline{x}'|}\mathrm{e}^{i\sqrt{\frac{z}{\alpha}}}$$

$$= \frac{m}{2\pi\hbar^2\,|\underline{x}-\underline{x}'|}\mathrm{e}^{\frac{i}{\hbar}\sqrt{2mz}|\underline{x}-\underline{x}'|}$$

(iii) Choosing $m = \frac{\hbar^2}{2}$ and $z = k^2$ we get the Greens function for $-\Delta + k^2$:

$$G(x,x') = \frac{1}{4\pi\,|\underline{x}-\underline{x}'|}\mathrm{e}^{i|k||\underline{x}-\underline{x}'|}$$

(iv) In one dimension the integral to solve becomes

$$G(x,x';z) = \int_{-\infty}^{+\infty}\frac{\mathrm{d}p}{2\pi\hbar}\frac{\mathrm{e}^{\frac{i}{\hbar}p(x-x')}}{\frac{p^2}{2m}-z} = \frac{1}{2\pi\,|x-x'|}\int_{-\infty}^{+\infty}\mathrm{d}q\frac{\mathrm{e}^{iq}}{\alpha q^2 - z}$$

The same replacements as in (ii) have been made and we can just repeat the steps from (ii) with the only difference that we have to close the integration contour above the real axis so that the exponential vanishes at complex infinity. The result is then:

$$G(x,x';z) = \frac{i}{2\sqrt{\alpha z}\,|x-x'|}\mathrm{e}^{i\sqrt{z/\alpha}} = \frac{i}{\hbar}\sqrt{\frac{m}{2z}}\mathrm{e}^{\frac{i}{\hbar}\sqrt{2mz}|x-x'|}$$

which diverges when we take the limit $z \to 0$

(v) First we start with a Laurent expansion of $G(x,x';z)$:

$$G(x,x';z) = \frac{i}{\hbar}\sqrt{\frac{m}{2z}} - \frac{m}{\hbar^2}\,|x-x'| + \mathscr{O}(\sqrt{z})$$

The higher order terms in $\sqrt{z}$ vanish in the limit $z \to 0$. Then the modified Greens function can be written as:

$$G(x,x') = \lim_{z\to 0}\left[-\sum_{i=-\infty}^{-2}A_i(\sqrt{z})^i + \frac{1}{\sqrt{z}}\left(\frac{i}{\hbar}\sqrt{\frac{m}{2}} - A_{-1}\right) - \frac{m}{\hbar^2}\,|x-x'| - A_0 + \mathscr{O}(\sqrt{z})\right]$$

For the limit to be well defined we choose $A_i = 0$ for $i \in]-\infty,-2]$ and $A_{-1} = \frac{i}{\hbar}\sqrt{\frac{m}{2}}$. As all the higher order coefficient do not contribute in the limit we can set them all to 0. To fix the form of A_0 we require that $G(x,x')$ is still a Greens function of $\hat{H}_0$:

$$-\frac{\hbar^2}{2m}\partial_x^2 G(x,x') = \frac{1}{2}\partial_x^2\,|x-x'| + \frac{\hbar^2}{2m}A_0'' = \delta(x-x') + \frac{\hbar^2}{2m}A_0''$$

Therefore A_0 must be of the form $A_0 = ax + b$.

(vi) Using solution from (v) we can write $\phi(x)$ as:

$$\phi(x) = \frac{1}{2}\int \mathrm{d}x'(|x - x'| + 2ax + 2b)f(x')$$

Now we apply the boundary condition. As $f(x)$ has only compact support in $[0, L]$ the limit $x \to -\infty$ becomes:

$$\lim_{x\to-\infty} \phi(x) = \frac{1}{2}\int \mathrm{d}x'(|x| - 2a\,|x| + b)f(x') \overset{!}{=} 0$$
$$\Rightarrow a = \frac{1}{2}; \qquad b = 0$$
$$\Rightarrow G(x, x') = -\frac{1}{2}(|x - x'| + x)$$

Exercise 50

Using the definitions given in the lecture, calculate the differential cross section $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ and the total cross section σ_{tot} for the Yukawa potential:

$$V(r) = \frac{V_0 \mathrm{e}^{-r/\alpha}}{r} \tag{6}$$

Check your result by taking the limit $\alpha \to \infty$. For the differential cross section you should get the Rutherford cross section.

Solution:

In the lecture the following formula for the differential cross section was derived:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int \mathrm{e}^{\frac{i}{\hbar}\underline{k}\underline{r}} V(\underline{r})\mathrm{d}^3 r\right|^2$$

$V(\underline{r})$ is the potential term in the Hamiltonian and $\underline{k} = \underline{p} - \underline{p}'$ is the momentum transfer. In an elastic scattering process, which we assume here, we have $|\underline{k}| = 2\,|\underline{p}| \sin\frac{\theta}{2}$, where θ is the scattering angle. Equipped with this we can now calculate the differential cross section for the Yukawa potential:

$$\begin{aligned}
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{m^2}{4\pi^2\hbar^4}\left|\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\int_0^{\infty}\mathrm{d}r r^2\sin\theta \mathrm{e}^{\frac{i}{\hbar}kr\cos\theta}\frac{V_0\mathrm{e}^{-r/\alpha}}{r}\right|^2 \\
&= \frac{m^2}{\hbar^4}\left|\int_{-1}^{+1}\mathrm{d}u\int_0^{\infty}\mathrm{d}r r\mathrm{e}^{\frac{i}{\hbar}kru}V_0\mathrm{e}^{-r/\alpha}\right|^2 = \frac{4V_0^2m^2}{k^2\hbar^2}\left|\int_0^{\infty}\mathrm{d}r\sin\left(\frac{kr}{\hbar}\right)\mathrm{e}^{-r/\alpha}\right|^2 \\
&= \frac{4V_0^2m^2}{k^2\hbar^2}\left|\int_0^{\infty}\mathrm{d}r\frac{1}{2i}\left(\mathrm{e}^{r(ik/\hbar-1/\alpha)} - \mathrm{e}^{-r(ik/\hbar+1/\alpha)}\right)\right|^2 = \frac{V_0^2m^2}{k^2\hbar^2}\left|\frac{-1}{ik/\hbar-1/\alpha} - \frac{1}{ik/\hbar+1/\alpha}\right|^2 \\
&= \frac{4V_0^2m^2\alpha^4}{(\alpha^2k^2+\hbar^2)^2} = \frac{4V_0^2m^2\alpha^4}{(4\alpha^2p^2\sin^2\theta/2+\hbar^2)^2}
\end{aligned}$$

Taking the limit $\alpha \to \infty$, we get:

$$\lim_{\alpha\to\infty}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \lim_{\alpha\to\infty}\frac{4V_0^2m^2\alpha^4}{\alpha^4(4p^2\sin^2\theta/2+\frac{\hbar^2}{\alpha^2})^2} = \frac{V_0^2m^2}{4p^4\sin^4\theta/2}$$

The total cross section can be obtained by integrating over the unit sphere:

$$\begin{aligned}
\sigma_{tot} &= \iint \mathrm{d}\phi\mathrm{d}\theta\sin\theta\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 8\pi V_0^2m^2\alpha^4\int_0^{\pi}\mathrm{d}\theta\frac{\sin\theta}{(4p^2\alpha^2\sin^2\theta/2+\hbar^2)^2} = 8\pi V_0^2m^2\alpha^4\int_{-1}^{+1}\mathrm{d}u\frac{1}{(2p^2\alpha^2(1-u)+\hbar^2)^2} \\
&= 8\pi V_0^2m^2\alpha^4\left[\frac{1}{2p^2\alpha^2(2p^2\alpha^2(1-u)+\hbar^2)}\right]_{-1}^{+1} = \frac{16\pi V_0^2m^2\alpha^4}{\hbar^2(4p^2\alpha^2+\hbar^2)}
\end{aligned}$$

Exercise 51 (central tutorial)

Consider the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V} = \frac{\hat{p}^2}{2m} + \lambda\delta(x)$. The eigenstates $|\, k\rangle$ with eigenvalue $\frac{k^2}{2m}$ of this Hamiltonian are given by

$$|\, k\rangle = \left|\, \bar{k}\right\rangle - \frac{1}{\hat{H}_0 - \frac{k^2}{2m} - i\epsilon}\hat{V}\,|\, k\rangle \tag{7}$$

where $\left|\, \bar{k}\right\rangle$ are the eigenstates of the free Hamiltonian with $\left\langle x \,|\, \bar{k}\right\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{i}{\hbar}xk}$.

(i) Using the result for the resolvent in one dimension from Exercise 49 calculate $\langle x\,|\,k\rangle$.

(ii) $|\, k\rangle$ as a function in k has a simple pole. Find the position k_0 of this pole and evaluate the residue $|\,\Psi\rangle := \mathrm{Res}_{k=k_0}\left\{|\, k\rangle\right\}$ of it.

(iii) Show that for $\lambda < 0$, $|\,\Psi\rangle$ is a bound state (normalizable eigenstate) of $\hat{H}$.

(iv) Extract the transmission and reflection coefficients from the explicit expression of $|\, k\rangle$.

Solution:

(i)

$$\langle x\,|\,k\rangle = \left\langle x\,|\,\bar{k}\right\rangle - \left\langle x \,\middle|\, \frac{1}{\hat{H}_0 - \frac{k^2}{2m} - i\epsilon}\hat{V} \,\middle|\, k\right\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{i}{\hbar}kx} - \int \mathrm{d}x' \left\langle x \,\middle|\, \frac{1}{\hat{H}_0 - \frac{k^2}{2m} - i\epsilon} \,\middle|\, x'\right\rangle \left\langle x' \,\middle|\, \hat{V} \,\middle|\, k\right\rangle$$

Now we can use the result from Exercise 49 (iv) with $z = \frac{k^2}{2m} + i\epsilon$ and take the limit $\epsilon \to 0$. Then the integral becomes:

$$\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{i}{\hbar}kx} - \frac{im}{\hbar k}\int \mathrm{d}x' \mathrm{e}^{\frac{i}{\hbar}k|x-x'|}\,\langle x'\,|\,\lambda\delta(x')\,|\,k\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{i}{\hbar}kx} - \frac{i\lambda m}{\hbar k}\mathrm{e}^{\frac{i}{\hbar}k|x-x'|}\,\langle 0\,|\,k\rangle$$

To calucalte $\langle 0\,|\,k\rangle$ we apply $\langle 0|$ to (7):

$$\begin{aligned}
\langle 0\,|\,k\rangle = \left\langle 0\,|\,\bar{k}\right\rangle - \left\langle 0 \,\middle|\, \frac{1}{\hat{H}_0 - \frac{k^2}{2m} - i\epsilon}\hat{V} \,\middle|\, k\right\rangle &= \frac{1}{\sqrt{2\pi\hbar}} - \frac{i\lambda m}{\hbar k}\,\langle 0\,|\,k\rangle \\
\Leftrightarrow \langle 0\,|\,k\rangle &= \frac{1}{\sqrt{2\pi\hbar}\left(1 + \frac{i\lambda m}{\hbar k}\right)} \\
\Rightarrow \langle x\,|\,k\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\left(\mathrm{e}^{\frac{i}{\hbar}kx} - \frac{i\lambda m}{\hbar k + i\lambda m}\mathrm{e}^{\frac{i}{\hbar}k|x|}\right)
\end{aligned}$$

(ii) To find the position of the pole we have to write $|\, k\rangle$ as a function in k:

$$|\, k\rangle = \int \mathrm{d}x\,\langle x\,|\,k\rangle\,|\,x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int \mathrm{d}x\left(\mathrm{e}^{\frac{i}{\hbar}kx} - \frac{i\lambda m}{\hbar k + i\lambda m}\mathrm{e}^{\frac{i}{\hbar}k|x|}\right)|\,x\rangle$$

In this form it becomes clear that $|\, k\rangle$ has a simple pole at $k_0 = -\frac{i\lambda m}{\hbar}$. So $|\,\Psi\rangle$ is given by:

$$\begin{aligned}
|\,\Psi\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\mathrm{Res}_{k=-\frac{i\lambda m}{\hbar}}\left\{\int \mathrm{d}x\left(\mathrm{e}^{\frac{i}{\hbar}kx} - \frac{1}{\hbar}\frac{i\lambda m}{k + \frac{i\lambda m}{\hbar}}\mathrm{e}^{\frac{i}{\hbar}k|x|}\right)|\,x\rangle\right\} \\
&= \frac{1}{\sqrt{2\pi\hbar}}\lim_{k\to -\frac{i\lambda m}{\hbar}}\left(\int \mathrm{d}x\left(\mathrm{e}^{\frac{i}{\hbar}kx} - \frac{1}{\hbar}\frac{i\lambda m}{k + \frac{i\lambda m}{\hbar}}\mathrm{e}^{\frac{i}{\hbar}k|x|}\right)(k + \frac{i\lambda m}{\hbar})\,|\,x\rangle\right) = -\frac{i\lambda m}{\sqrt{2\pi\hbar^3}}\int \mathrm{d}x\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}}\,|\,x\rangle
\end{aligned}$$

(iii) First we need to show that $|\,\Psi\rangle$ is an eigenstate of $\hat{H}$:

$$\begin{aligned}
\left\langle x \,\middle|\, \hat{H} \,\middle|\, \Psi\right\rangle &= \left(-\frac{\hbar^2}{2m}\partial_x^2 + \lambda\delta(x)\right)\langle x\,|\,\Psi\rangle = \left(-\frac{\hbar^2}{2m}\partial_x^2 + \lambda\delta(x)\right)\left(-\frac{i\lambda m}{\sqrt{2\pi\hbar^3}}\right)\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}} \\
&= \frac{i\lambda m}{\sqrt{2\pi\hbar^3}}\left(\frac{\hbar^2}{2m}\partial_x^2\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}} - \lambda\delta(x)\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}}\right) = \frac{i\lambda m}{\sqrt{2\pi\hbar^3}}\left(\frac{\hbar^2}{2m}\partial_x\left(\frac{\lambda m}{\hbar^2}\,\mathrm{sgn}(x)\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}}\right) - \lambda\delta(x)\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}}\right) \\
&= \frac{i\lambda m}{\sqrt{2\pi\hbar^3}}\left(\frac{\hbar^2}{2m}\left(\frac{\lambda m}{\hbar^2}2\delta(x) + \left(\frac{\lambda m}{\hbar^2}\right)^2\mathrm{sgn}^2(x)\right)\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}} - \lambda\delta(x)\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}}\right) = \frac{i\lambda m}{\sqrt{2\pi\hbar^3}}\left(\frac{1}{2}\frac{m\lambda^2}{\hbar^2}\mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}}\right) \\
&= -\frac{1}{2}\frac{m\lambda^2}{\hbar^2}\,\langle x\,|\,\Psi\rangle
\end{aligned}$$

Now we can calculate the norm of $|\,\Psi\rangle$:

$$\||\,\Psi\rangle\| = \int \mathrm{d}x\,|\langle x\,|\,\Psi\rangle|^2 = \int \mathrm{d}x \left| -\frac{i\lambda m}{\sqrt{2\pi\hbar^3}} \mathrm{e}^{\frac{\lambda m|x|}{\hbar^2}} \right|^2 = \frac{m^2\lambda^2}{2\pi\hbar^3} \int_{-\infty}^{+\infty} \mathrm{d}x \mathrm{e}^{2\frac{\lambda m|x|}{\hbar^2}}$$
$$= \frac{m^2\lambda^2}{\pi\hbar^3} \left[\frac{\hbar^2}{2m\lambda} \mathrm{e}^{2\lambda m x} \right]_0^\infty$$

It is clear that this is only finite for $\lambda < 0$.

(iv) We can seperate $\langle x\,|\,k\rangle$ into two parts for $x < 0$ and $x > 0$:

$$\langle x\,|\,k\rangle = \begin{cases} \frac{1}{\sqrt{2\pi\hbar}} \frac{\hbar k}{\hbar k + i\lambda m} \mathrm{e}^{\frac{i}{\hbar}kx} & \text{for } x > 0 \\ \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{\frac{i}{\hbar}kx} - \frac{i\lambda m}{\sqrt{2\pi\hbar}(\hbar k + i\lambda m)} \mathrm{e}^{-\frac{i}{\hbar}kx} & \text{for } x < 0 \end{cases}$$

We can interpret this as a free wave coming from $x \to -\infty$. Then the first term in the second line represents the in coming wave function $\psi_{in}(x)$, the second term is the reflected part of the wave function $\psi_R(x)$ and the first line is the transmitted part of the wave function $\psi_T(x)$. The transmission and reflection coefficients are given by:

$$\mathscr{T} = \frac{|\psi_T|^2}{|\psi_{in}|^2} = \frac{\hbar^2 k^2}{\hbar^2 k^2 + \lambda^2 m^2}$$
$$\mathscr{R} = \frac{|\psi_R|^2}{|\psi_{in}|^2} = \frac{\lambda^2 m^2}{\hbar^2 k^2 + \lambda^2 m^2}$$
$$\Rightarrow \mathscr{T} + \mathscr{R} = 1$$

Exercise 52

Consider the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$ in one dimension where the potential is given by

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases} \tag{8}$$

(i) Make the following ansatz for the wave function $\psi(x)$

$$\psi(x) = \begin{cases} A\mathrm{e}^{ik_1x} + B\mathrm{e}^{-ik_1x} & \text{for } x < 0 \\ C\mathrm{e}^{ik_2x} + D\mathrm{e}^{-ik_2x} & \text{for } x \geq 0 \end{cases} \tag{9}$$

and solve the time independent Schrödinger equation to get expressions for k_1 and k_2.

(ii) By matching the boundary conditions $\lim_{x\to0+} \psi(x) = \lim_{x\to0-} \psi(x)$ and $\lim_{x\to0+} \psi'(x) = \lim_{x\to0-} \psi'(x)$ find a relation between the coefficients A, B, C and D. Why do these boundary conditions make sense?

(iii) Find the transmission and reflection coefficient for a wave coming from $-\infty$.

Solution:

(i) Define the two different parts of the wave function as:

$$\psi_1(x) = A\mathrm{e}^{ik_1x} + B\mathrm{e}^{-ik_1x}$$
$$\psi_2(x) = C\mathrm{e}^{ik_2x} + D\mathrm{e}^{-ik_2x}$$

Pluggin this into the Scrödinger equation we get:

$$-\frac{\hbar^2}{2m}\partial_x^2\psi_1(x) = \frac{\hbar^2 k_1^2}{2m}\psi_1(x) = E\psi_1(x) \quad \Leftrightarrow k_1 = \frac{\sqrt{2mE}}{\hbar}$$
$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V_0\right)\psi_2(x) = \left(\frac{\hbar^2 k_1^2}{2m} + V_0\right)\psi_2(x) = E\psi_2(x) \quad \Leftrightarrow k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$
$$\Rightarrow k_2^2 = k_1^2 - \frac{2mV_0}{\hbar^2}$$

We see immediately that in the classically forbidden region of $E < V_0$ the wave function stops propagation but falls of exponentially. However there is still a nonvanishing expectation value (tunelling effect).

(ii) These boundary conditions make sense as the Schrödinger equation implies the continuity of the wave function and its first derivative which is what we implement by these boundary conditions.

$$\begin{aligned} \psi_1(0) = \psi_2(0) \quad &\Rightarrow A + B = C + D \\ \psi_1'(0) = \psi_2'(0) \quad &\Rightarrow k_1(A - B) = k_2(C - D) \end{aligned}$$

Solving this for A and B we get:

$$\begin{aligned} A &= \frac{1}{2}\left(\left(1 + \frac{k_2}{k_1}\right)C + \left(1 - \frac{k_2}{k_1}\right)D\right) \\ B &= \frac{1}{2}\left(\left(1 - \frac{k_2}{k_1}\right)C + \left(1 + \frac{k_2}{k_1}\right)D\right) \end{aligned}$$

(iii) Now we postulate that our wave function represents a free particle coming from $-\infty$. That means the only part which travels in the opposite direction must have been reflected from the potential. Therefore we can already fix the coefficients $A = \frac{1}{\sqrt{2\pi\hbar}}$ and $D = 0$.

$$\begin{aligned} \Rightarrow A = \frac{1}{\sqrt{2\pi\hbar}} &= \frac{1}{2}\left(1 + \frac{k_2}{k_1}\right)C \quad \Leftrightarrow C = \frac{1}{\sqrt{2\pi\hbar}}\frac{2k_1}{k_1 + k_2} \\ B &= \frac{1}{2}\left(1 - \frac{k_2}{k_1}\right)C \quad \Leftrightarrow B = \frac{1}{\sqrt{2\pi\hbar}}\frac{k_1 - k_2}{k_1 + k_2} \end{aligned}$$

The reflection coefficient are defined via the probalitity flux $j(x) = -\frac{i\hbar}{2m}(\psi^*\partial_x\psi - (\partial_x\psi^*)\psi)$ as:

$$\mathscr{R} = \frac{|j_R|}{|j_{in}|} \qquad \mathscr{T} = \frac{|j_T|}{|j_{in}|}$$

where j_{in}, j_R and j_T represent the probability flux for the in coming, the reflected and the transmitted wave respectively:

$$j_{in} = \frac{k_1}{2\pi m} \qquad j_R = -\frac{k_1}{2\pi m}\left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$j_T = \frac{k_2}{2\pi m}\frac{4k_1^2}{(k_1 + k_2)^2}$$

$$\mathscr{R} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$\mathscr{T} = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \Rightarrow \mathscr{R} + \mathscr{T} = 1$$