Moderne Physik für Lehramtskandidaten

Vorlesung: PD Dr. S. Gieseke – Übung: Dr. C. B. Duncan

Lösung 10

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Aufgabe 1: Unendlicher Potentialtopf (10 P)
Betrachten Sie ein Teilchen im folgenden eindimensionalen Potential

$$V(x) = \begin{cases} 0, & x \in [-a/2, a/2] \\ \infty, & \text{sonst} \end{cases}$$

wobei a die Breite des Potentialtopfes parametrisiert. Lösen Sie die stationäre Schrödingergleichung für $E > 0$

$$\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\Big]\psi(x) = E\psi(x)$$

Eine allgemeine Lösung der Wellengleichung ist gegeben durch

$$\psi(x) = \alpha e^{ikx} + \beta e^{-ikx}$$

wobei die Paramete α, β durch die Randbedingungen bestimmt werden können. Überlegen Sie sich dazu wie die Wellenfunktion außerhalb des Topfes aussehen und welche weitere Eigenschaften die Wellenfunktion erfüllen muss.

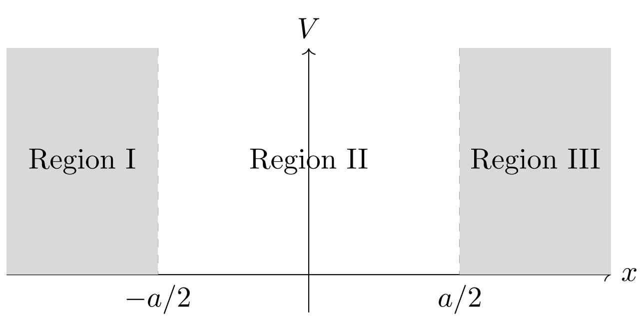
(a) Bestimmen Sie die Energieeigenwerte und die Wellenfunktionen und zeigen Sie dass die Energie *quantisiert* ist.

(b) Was passiert für Energien $E < 0$?

Solution to Aufgabe 1:
Infinite potential well described by the following potential:

$$V(x) = \begin{cases} 0, & x \in [-a/2, a/2] \\ \infty, & \text{sonst} \end{cases}$$

A sketch of the system:



(a) We begin by considering the positive energy case $E > 0$.
Recipe for potential problems:

1. Begin by dividing the problem into physical and unphysical areas. Here regions 1 and 3 are unphysical due to their infinite potential energies, while region 2 is the allowed space.

2. Ansätze for the different areas:

$$\psi_I(x) = \psi_{III}(x) = 0 \quad \forall x \in I, III$$
$$\psi_{II}(x) = \alpha e^{\mathrm{i}kx} + \beta e^{-\mathrm{i}kx}$$

   Region II is the physically allowed region, so we use the ansatz of plane waves, and there are two degrees of freedom.

3. Determining the energies:

   We use the Schrödinger equation:

$$\Big[-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\Big]\psi(x) = E\psi(x)$$
$$\Leftrightarrow \hat{S}\psi(x) = 0$$
$$\text{where } \hat{S} = -\frac{\hbar^2}{2m}\partial_x^2 + V(x) - E$$

   Applying this operator $\hat{S}$ to the wavefunction in region II:

$$\hat{S}\psi_{II}(x) = 0$$
$$\Rightarrow -\frac{\hbar^2}{2m}\big((\mathrm{i}k)^2\alpha e^{\mathrm{i}kx} + (-\mathrm{i}k)^2\beta e^{-\mathrm{i}kx}\big) + 0 - E\psi_I I(x) = 0$$
$$\Rightarrow \Big(-\frac{\hbar^2}{2m}(\mathrm{i}k)^2 - E\Big)\psi(x) = 0 \quad \forall x \in \mathbb{R}$$
$$\Rightarrow k^2 = \frac{2mE}{\hbar^2} \quad \forall\, x \in \text{ Region II}$$

   k would become imaginary for $E < 0$!

4. Determination of the free parameters by using the boundary conditions/constraints.

   Things we know about the wavefunction

   - $\psi(x)$ is continuous.
   - $\psi(x)$ is differentiable.
   - $\int \mathrm{d}x|\psi(x)|^2 = 1$ - conservation of unit probability.

   (i) Using the first quality (continuity):

$$\psi_I(x = -a/2) \stackrel{!}{=} \psi_{II}(x = -a/2)$$
$$\Leftrightarrow 0 = \alpha e^{-\mathrm{i}ka/2} + \beta e^{\mathrm{i}ka/2} - (1)$$

   Similarly on the other side:

$$\psi_{II}(x = a/2) \stackrel{!}{=} \psi_{III}(x = a/2)$$
$$\Leftrightarrow 0 = \alpha e^{\mathrm{i}ka/2} + \beta e^{-\mathrm{i}ka/2} - (2)$$

Rewriting (1) and (2) and subtracting:

$$\begin{aligned} \alpha + \beta e^{\mathrm{i}ka} &= 0 \\ \alpha + \beta e^{-\mathrm{i}ka} &= 0 \\ \Rightarrow \beta\big(e^{\mathrm{i}ka} - e^{-\mathrm{i}ka}\big) &= 0 \end{aligned}$$

So we could have the solutions $\beta = 0$, but then $\alpha = 0$, i.e. the wavefunction is trivially 0 everywhere. The other solution is that:

$$\begin{aligned} 2\mathrm{i}\beta \sin(ka) &= 0 \\ \Rightarrow ka &= n\pi, \quad n \in \mathbb{Z} \end{aligned}$$

and using $k = \sqrt{2mE/\hbar}$, the energy levels are given by:

$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2, \quad n \in \mathbb{Z}$$

i.e. we have quantized energy levels! What do the energy levels look like?

The question now is: what is α? Adding (1) and (2):

$$\begin{aligned} \alpha &= -\beta \\ \Rightarrow \psi_{II}(x) &= \alpha\big(e^{\mathrm{i}kx} - e^{-\mathrm{i}kx}\big) \\ &= 2\mathrm{i}\alpha \sin kx \\ &= \tilde{\alpha} \sin\big(n\pi x/a\big) \end{aligned}$$

where the $\tilde{\alpha}$ is still a free parameter.

(ii) Now we can use the normalization condition:

$$\begin{aligned} \int \mathrm{d}x|\psi|^2 &= \int_{-a/2}^{a/2} \mathrm{d}x|\psi_{II}(x)|^2 \\ &= \int_{-a/2}^{a/2} |\tilde{\alpha}|^2 \sin^2 kx \\ &= |\tilde{\alpha}|^2\Big(\frac{a}{2} - \frac{\sin ka}{2k}\Big) \end{aligned}$$

The second term on the last line will always be zero ($ka = n\pi \Rightarrow \sin ka = 0$), so we finally have:

$$\begin{aligned} 1 &= |\tilde{\alpha}|^2\frac{a}{2} \\ \Rightarrow \tilde{\alpha} &= \sqrt{2/a} \end{aligned}$$

Thus, overall, we have a wavefunction that looks like:

$$\psi(x) = \begin{cases} 0, & x \in I \\ \sqrt{2/a}\sin kx, & x \in II \\ 0, & x \in III \end{cases}$$

with energy levels given by:

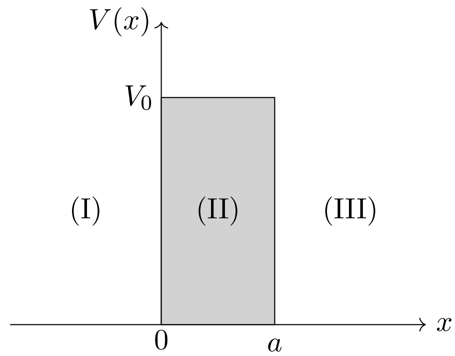
$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

i.e. we have quantized energies of standing waves.

(b) For the case of negative energy $E < 0$, the negative energy solutions are unphysical and there are no such particles that can exist.

N.B. The eigenvalues, i.e. the energies E_n of the potential well should be the same regardless of the choice of coordinates, but note that $\psi(x)$ does change. This is because the translation introduces a phase-shift, which is not observable (upon taking the mod-square of the wavefunction, it yields unity).

Aufgabe 2: Tunneleffekt (7 P)



Betrachten Sie eine kastenförmige Potentialbarriere der Höhe V_0. Das Ziel: Die Berechnung der stationären Zustände eines Teilchens der Energie $E < V_0$, welches sich auf die Barriere zubewegt und die Bestimmung dadurch den Transmissionskoeffizienten $t = t(E)$.

(a) **(2 P)** Benutzen Sie die folgenden Ansätze für die Wellenfunktion in den drei Bereichen $(I), (II)$ und (III):

$$\begin{aligned} \psi_I(x) &= e^{\mathrm{i}kx} + re^{-\mathrm{i}kx}, \\ \psi_{II}(x) &= pe^{\kappa x} + qe^{-\kappa x}, \\ \psi_{III}(x) &= te^{\mathrm{i}k(x-a)}. \end{aligned}$$

Mit Hilfe der stationären Schrödingergleichung berechnen Sie die Parametern k und κ als Funktionen der Energie E und Potenzial V_0.

(b) **(4 P)** Verwenden Sie für die Randbedingungen zwischen den drei Bereichen nun die Stetigkeit der Wellenfunktion und deren Ableitung, um daraus die Koeffizienten r, t in den Formen

$$\begin{aligned} t &= \frac{2ik\kappa}{2ik\kappa \cosh \kappa a + (k^2 - \kappa^2) \sinh \kappa a} \\ r &= \frac{(\kappa^2 + k^2) \sinh \kappa a}{2ik\kappa \cosh \kappa a + (k^2 - \kappa^2) \sinh \kappa a} \end{aligned}$$

bringen zu können.

(c) **(1 P)** Beschreiben Sie qualitativ, was mit r und t passiert, wenn $a \to 0$ und $a \to \infty$?

Solution to Aufgabe 2:

We're going to consider the situation where $0 < E < V_0$, i.e. classically, region II is physically forbidden. Since we are using quantum mechanics, we will use the (one-dimensional, time-independent) Schrödinger equation (TISE):

$$\left[-\frac{\hbar^2}{2m}\partial_x^2 + V(x) - E \right] \psi(x) = 0$$

with the Ansätze:

$$\psi_I(x) = e^{\mathrm{i}kx} + re^{-\mathrm{i}kx},$$
$$\psi_{II}(x) = pe^{\kappa x} + qe^{-\kappa x},$$
$$\psi_{III}(x) = te^{\mathrm{i}k(x-a)}$$

Note that the wavefunction for region II is an exponential is because it is a classically forbidden region.

Derivatives:

$$\psi'_I(x) = ik\big(e^{\mathrm{i}kx} - re^{-\mathrm{i}kx}\big)$$
$$\psi'_{II}(x) = \alpha\big(pe^{\kappa x} - qe^{-\kappa x}\big)$$
$$\psi'_{III}(x) = ikte^{\mathrm{i}k(x-a)}$$

Calculating the energy by substituting into the TISE:

$$(I) \rightarrow \big(-\frac{\hbar^2}{2m}(ik)^2 + 0 - E\big)\psi_I(x) = 0 \quad \Rightarrow k^2 = \frac{2mE}{\hbar^2}$$
$$(II) \rightarrow \big(-\frac{\hbar^2}{2m}(\kappa)^2 + V_0 - E\big)\psi_{II}(x) = 0 \quad \Rightarrow \kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

Region III has the same energy eigenvalues as region I.

Continuity:

$$\text{For } x = 0: \quad 1 + r = p + q \quad \leftarrow (1)$$
$$\text{For } x = a: \quad pe^{\kappa a} + qe^{-\kappa a} = t \quad \leftarrow (2)$$

Continuity of derivative:

$$\text{For } x = 0: \quad ik(1 - r) = \kappa(p - q) \quad \leftarrow (3)$$
$$\text{For } x = a: \quad \kappa\big(pe^{\kappa a} - qe^{-\kappa a}\big) = ikt \quad \leftarrow (4)$$

We want to find the transmission and reflection coefficients t, r. Substituting Eq.(2) into Eq. (4):

$$qe^{-\kappa a} = t - pe^{\kappa a}$$
$$ikt = \kappa\big(pe^{\kappa a} - (t - pe^{\kappa a})\big)$$
$$\Rightarrow t = \frac{2\kappa}{ik + \kappa}pe^{\kappa a}$$

But what about p? Is that non-zero?

First, consider the combination $ik \cdot (1) + (3)$:

$$ik(1 + r + 1 - r) = (ik + \kappa)p + q(ik - \kappa)$$
$$\Rightarrow 0 = p(ik + \kappa) + q(ik - \kappa) - 2ik \quad \leftarrow (5)$$

For the combination $ik \cdot (2) - (4)$:

$$p(ik - \kappa)e^{\kappa a} + q(ik + \kappa)e^{-\kappa a} = 0 \quad \leftarrow (6)$$

Now, taking the combination $-(ik + \kappa)e^{-\kappa a} \cdot (5) + (ik - \kappa) \cdot (6)$:

$$-p(ik + \kappa)^2 e^{-\kappa a} - (ik - \kappa)(ik + \kappa)e^{-\kappa a}q + 2ik(ik + \kappa)e^{-\kappa a}$$
$$+p(ik - \kappa)^2 e^{\kappa a} + q(ik + \kappa)(ik - \kappa)e^{-\kappa a} = 0$$

Notice that the terms with q cancel. Rearranging:

$$p\big((k^2-\kappa^2+2ik\kappa)e^{\kappa a}+(-k^2+\kappa^2+2ik\kappa)e^{-\kappa a}\big)=2ik(ik+\kappa)e^{-\kappa a}$$
$$\Rightarrow p\big((k^2-\kappa^2)(e^{\kappa a}-e^{-\kappa a})+2ik\kappa(e^{\kappa a}+e^{-\kappa a})\big)=2ik(ik+\kappa)e^{-\kappa a}$$

Using the fact that $e^{\kappa a}-e^{-\kappa a}=2\sinh(\kappa a)$ and $e^{\kappa a}+e^{-\kappa a}=2\cosh(\kappa a)$:

$$pe^{\kappa a}=\frac{ik(ik+\kappa)}{2ik\kappa\cosh(\kappa a)+(k^2-\kappa^2)\sinh(\kappa a)}\quad\leftarrow(7)$$

i.e. p is in general non-zero, meaning that t (reminder, given by):

$$t=\frac{2\kappa}{ik+\kappa}e^{\kappa a}p\quad\leftarrow(8)$$

will also in general be non-zero, i.e. the wavefunction on the other side of the barrier is non-zero, i.e. there is transmission through the wall. In other words, there is a non-zero probability ($|\psi|^2$) of finding the particle on the other side of the wall. This phenomenon is known as **(quantum) tunneling**.

Inserting Eq. (7) into Eq. (8) yields the identity for the transmission coefficient:

$$t=\frac{2ik\kappa}{2ik\kappa\cosh\kappa a+(k^2-\kappa^2)\sinh\kappa a}$$

For the reflection coefficient, take the linear combination $ik(1)-(3)$:

$$\Rightarrow p(ik-\kappa)+q(ik-\kappa)-2ikr=0\quad\leftarrow(9)$$

Now, using the combination $e^{-\kappa a}(9)-(6)$:

$$pe^{-\kappa a}(ik-\kappa)+qe^{-\kappa a}(ik+\kappa)-2ikre^{-\kappa a}-pe^{\kappa a}(ik-\kappa)-qe^{-\kappa a}(ik+\kappa)=0$$

Notice that the q terms cancel again:

$$p(ik-\kappa)\big(e^{-\kappa a}-e^{\kappa a}\big)=2ikre^{-\kappa a}$$
$$\Rightarrow r=\frac{(\kappa-ik)\sinh\kappa a}{ik}pe^{\kappa a}$$
$$=\frac{(\kappa-ik)\sinh\kappa a}{ik}\frac{ik(ik+\kappa)}{2ik\kappa\cosh(\kappa a)+(k^2-\kappa^2)\sinh(\kappa a)}$$
$$=\frac{(\kappa^2+k^2)\sinh\kappa a}{2ik\kappa\cosh\kappa a+(k^2-\kappa^2)\sinh\kappa a}$$

Considering the limits $a\to 0$ and $a\to\infty$, we can rewrite the transmission and reflection coefficients as

$$t=\frac{2ik\kappa}{\Big[2ik\kappa+(k^2-\kappa^2)\tanh\kappa a\Big]\cosh\kappa a}$$
$$r=\frac{(\kappa^2+k^2)\sinh\kappa a}{\Big[2ik\kappa+(k^2-\kappa^2)\tanh\kappa a\Big]\cosh\kappa a}$$

i.e. there isn't a transmission coefficient into 'free space' because there is no free space. Instead p will become the new t, and is in general non-zero, since as we can see, r is in general non-zero.

In the limit of $a\to\infty$, $\tanh\kappa a\to 1$, so

$$t\to\frac{2ik\kappa}{2ik\kappa+(k^2-\kappa^2)}\frac{1}{\cosh\kappa a}\to 0$$
$$r\to\frac{(\kappa+ik)(\kappa-ik)}{(ik-\kappa)(\kappa-ik)}=\frac{ik+\kappa}{ik-\kappa}$$

where $\cosh \kappa a \to \infty$ in this limit.

In the other limit $a \to 0$, $\cosh \kappa a \to 1$ and $\sinh \kappa a \to 0$:

$$\begin{aligned} t &\to \frac{2ik\kappa}{2ik\kappa} = 1 \\ r &\to 0 \end{aligned}$$

Aufgabe 3: (5 P) Atomare Bindung

Betrachten Sie ein Elektron im eindimensionalen Potential

$$V(x) = \begin{cases} \infty & \text{für } \ x < 0 \\ 0 & \text{für } \ 0 \le x < a \\ V_0 > 0 & \text{für } \ x > a \end{cases}$$

Sei die Energie des Elektrons $E < V_0$ und die Masse m.

(a) **(1 P)** Gegeben Sie die Wellenfunktion

$$\psi(x) = \begin{cases} 0 & \text{für } \ x < 0 \\ Ae^{ikx} + Be^{-ikx} & \text{für } \ 0 \le x < a \ , \\ Ce^{\kappa(x-a)} + De^{-\kappa(x-a)} & \text{für } \ x > a \end{cases}$$

bestimmen Sie k und κ als Funktion von E, m und V_0.

(b) **(2 P)** Zeigen Sie, dass C Null sein muss. Bestimmen Sie die Koeffizienten A und B als Funktion von D, k, κ und a.

(c) **(1 P)** Zeigen Sie, dass die folgende Gleichung

$$\tan(ka) = -\frac{k}{\kappa}$$

gilt.

(d) **(1 P)** Wie hoch muss V_0 mindestens sein, damit ein gebundener Zustand vorliegt?

Hinweis: Ist es möglich, eine reelle Lösung für die obige Gleichung zu finden, wenn $0 < ka < \pi/2$? Denken Sie danach, was größer ist: E oder V_0?

Lösung 5:

(a) **(1 P)** First derivative of wavefunction:

$$\psi'(x) = \begin{cases} 0 & \text{für } \ x < 0 \\ ik(Ae^{ikx} - Be^{-ikx}) & \text{für } \ 0 \le x < a \ , \\ \kappa(Ce^{\kappa(x-a)} - De^{-\kappa(x-a)}) & \text{für } \ x > a \end{cases}$$

Second derivative:

$$\psi''(x) = \begin{cases} 0 & \text{für } \ x < 0 \\ -k^2(Ae^{ikx} + Be^{-ikx}) & \text{für } \ 0 \le x < a \ , \\ \kappa^2(Ce^{\kappa(x-a)} + De^{-\kappa(x-a)}) & \text{für } \ x > a \end{cases}$$

Time-independent Schrödinger equation:

$$\text{For } \ 0 < x < a: \ -\frac{\hbar^2}{2m}(-k^2\psi) + 0 = E\psi \qquad \Rightarrow k = \sqrt{\frac{2mE}{\hbar^2}}$$
$$\text{For } \ a < x: \ -\frac{\hbar^2}{2m}(\kappa^2\psi) + V_0\psi = E\psi \qquad \Rightarrow \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

(b) **(2 P)** First, to show that $C = 0$, the wavefunction must vanish as we go to infinity

$$\psi_{III}(x) \overset{x\to\infty}{\to} 0$$

The exponent for the D term will vanish, but C's exponent will diverge, meaning that to keep the wavefunction finite, $C = 0$.

For the other coefficients, we use the continuity of the wavefunction:

$$\psi_I(0) = \psi_{II}(0) \quad \Rightarrow 0 = A + B \quad \Rightarrow \boxed{A = -B}$$
$$\psi_{II}(a) = \psi_{III}(a) \quad \Rightarrow Ae^{ika} + Be^{ika} = D \quad \Rightarrow \boxed{2Ai\sin(ka) = D}$$
$$\Rightarrow A = \frac{D}{2i\sin(ka)} = -B$$

Continuity of the first derivative of the wavefunction:

$$\psi'_{II}(a) = \psi'_{III}(a) \quad \Rightarrow \boxed{ikA\big(e^{ika} + e^{-ika}\big) = -\kappa D}$$
$$2ikA\cos(ka) = -\kappa D$$

(c) **(1 P)** Using the last two results to remove D, we see:

$$A = \frac{D}{2i\sin(ka)} = -\frac{2ikA\cos(ka)}{2i\kappa\sin(ka)}$$
$$\Rightarrow A = -A\frac{k\cos(ka)}{\kappa\sin(ka)}$$
$$\Rightarrow 1 = -\frac{k}{\kappa}\frac{1}{\tan(ka)}$$
$$\Rightarrow \tan(ka) = -\frac{k}{\kappa}$$

(d) **(1 P)** The left hand side of the equation is positive for $0 \leq ka < \pi/2$, while it will always be negative on the right hand side. So we only have *at least one* solution when:

$$ka > \frac{\pi}{2}$$
$$k = \sqrt{\frac{2mE}{\hbar^2}} > \frac{\pi}{2a}$$
$$\Rightarrow E > \frac{\pi^2\hbar^2}{8ma^2}$$

and since we have $E < V_0$, the minimum value for V_0 needed for a bounded state is:

$$V_0 > \frac{\pi^2\hbar^2}{8ma^2}$$