Moderne Physik für Lehramtskandidaten

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Lösung 11

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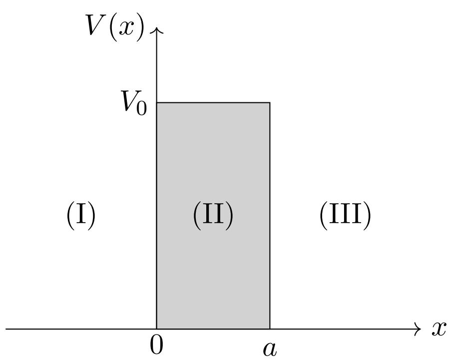
Aufgabe 1: Tunneleffekt (12 P)



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

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

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

(b) **(6 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

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

bringen zu können.

(c) **(2 P)** Beschreiben Sie qualitativ, was mit r und t passiert, wenn $a \to 0$ und $a \to \infty$?

Solution to Aufgabe 1:

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):

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

with the Ansätze:

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

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

Derivatives:

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

Calculating the energy by substituting into the TISE:

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

Region III has the same energy eigenvalues as region I.

Continuity:

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

Continuity of derivative:

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

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

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

But what about p? Is that non-zero?

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

$$\begin{aligned}ik(1 + r + 1 - r) &= (ik + \kappa)p + q(ik - \kappa)\\ \Rightarrow 0 &= p(ik + \kappa) + q(ik - \kappa) - 2ik \quad \leftarrow (5)\end{aligned}$$

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 $-(ik+\kappa)e^{-\kappa a} \cdot (5) + (ik-\kappa)\cdot(6)$:

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

Notice that the terms with q cancel. Rearranging:

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

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:

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

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

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

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 $\sinh \kappa a \to 0$:

$$t \to \frac{2ik\kappa}{2ik\kappa} = 1$$
$$r \to 0$$

Aufgabe 2: (8 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) **(2 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) **(2 P)** Zeigen Sie, dass die folgende Gleichung

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

gilt.

(d) **(2 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?

(a) **(2 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) **(2 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) **(2 P)** The left hand side of the equation is positive for $0 \le ka < \pi/2$, 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:

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