Kodutöö 7

Kvantmehaanika magistrikursus

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1. Arvutage joonisel kujutatud astmelise potentsiaali läbilaskvus- ja peegelduskoefitsiendid (T ja R), kasutades ülekandemaatriksi meetodit ning eeldades, et $E > V_2$.

Katkevusmaatriksid üleminekute $1 \to 2$ ja $2 \to 3$ jaoks:

$$D_{12} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_2}{k_1} & 1 - \frac{k_2}{k_1} \\ 1 - \frac{k_2}{k_1} & 1 + \frac{k_2}{k_1} \end{bmatrix} \tag{1}$$

$$D_{23} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_3}{k_2} & 1 - \frac{k_3}{k_2} \\ 1 - \frac{k_3}{k_2} & 1 + \frac{k_3}{k_2} \end{bmatrix} \tag{2}$$

Levikumaatriks piirkonna 2 jaoks:

$$P_2 = \begin{bmatrix} e^{-ik_2 a} & 0 \\ 0 & e^{ik_2 a} \end{bmatrix} \tag{3}$$

Ülekandemaatriks avaldub järgmiselt (algsesse koordinaadisüsteemi pole tarvis tagasi minna, kui meid huvitavad ainult läbilaskvus ja peegelduskoefitsient):

$$\begin{aligned} T_{13} = \begin{bmatrix} T_1 & T_3 \\ T_2 & T_4 \end{bmatrix} &= D_{12} P_2 D_{23} = \frac{1}{2} \begin{bmatrix} e^{-ik_2 a}\left(1 + \frac{k_2}{k_1}\right) & e^{ik_2 a}\left(1 - \frac{k_2}{k_1}\right) \\ e^{-ik_2 a}\left(1 - \frac{k_2}{k_1}\right) & e^{ik_2 a}\left(1 + \frac{k_2}{k_1}\right) \end{bmatrix} D_{23}, \\ T_1 &= \frac{1}{4}\left(e^{-ik_2 a}\left(1 + \frac{k_2}{k_1} + \frac{k_3}{k_2} + \frac{k_3}{k_1}\right) + e^{ik_2 a}\left(1 - \frac{k_2}{k_1} - \frac{k_3}{k_2} + \frac{k_3}{k_1}\right)\right) \\ &= \frac{1}{2}\left[\left(1 + \frac{k_3}{k_1}\right)\cos(k_2 a) - i\left(\frac{k_2}{k_1} + \frac{k_3}{k_2}\right)\sin(k_2 a)\right], \\ T_2 &= \frac{1}{4}\left(e^{-ik_2 a}\left(1 + \frac{k_2}{k_1} - \frac{k_3}{k_2} - \frac{k_3}{k_1}\right) + e^{ik_2 a}\left(1 - \frac{k_2}{k_1} + \frac{k_3}{k_2} - \frac{k_3}{k_1}\right)\right) \\ &= \frac{1}{2}\left[\left(1 - \frac{k_3}{k_1}\right)\cos(k_2 a) - i\left(\frac{k_2}{k_1} - \frac{k_3}{k_2}\right)\sin(k_2 a)\right]. \end{aligned} \tag{4}$$

Asendades $L_1 \equiv 1 + \frac{k_3}{k_1}$, $L_2 \equiv \frac{k_2}{k_1} + \frac{k_3}{k_2}$, $\alpha = ak_2$, saame

$$T_1 = \frac{1}{4}\left(e^{-i\alpha}(L_1 + L_2) + e^{i\alpha}(L_1 - L_2)\right) = \frac{1}{2}\left(L_1 \cos(\alpha) - iL_2 \sin(\alpha)\right). \tag{5}$$

Tehes ka asendused $L_3 \equiv 1 - \frac{k_3}{k_1}$, $L_4 \equiv \frac{k_2}{k_1} - \frac{k_3}{k_2}$, saame

$$T_2 = \frac{1}{2}\left(L_3 \cos(\alpha) - iL_4 \sin(\alpha)\right). \tag{6}$$

Arvestades, et levimine toimub suunas $1 \to 3$,

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = T_{13} \begin{bmatrix} A_3 \\ 0 \end{bmatrix} = \begin{bmatrix} T_1 A_3 \\ T_2 A_3 \end{bmatrix}, \tag{7}$$

kus A_i ja B_i on vastavalt regiooni i paremale poole ja vasakule poole liikuva exponendi koefitsiendid ($B_3 = 0$, kuna selles suunas ei peegeldu lainet).

Arvestades, et

$$j_{1\rightarrow} = |A_1|^2 \frac{\hbar k_1}{m}, \tag{8}$$

$$j_{1\leftarrow} = |B_1|^2 \frac{\hbar k_1}{m}, \tag{9}$$

$$j_{3\rightarrow} = |A_3|^2 \frac{\hbar k_3}{m}, \tag{10}$$

siis

$$T = \frac{j_{3\rightarrow}}{j_{1\rightarrow}} = \frac{|A_3|^2 k_3}{|A_1|^2 k_1} = \frac{k_3}{k_1} \frac{1}{|T_1|^2}, \tag{11}$$

$$R = \frac{j_{1\leftarrow}}{j_{1\rightarrow}} = \frac{|B_1|^2}{|A_1|^2} = \frac{|T_2|^2}{|T_1|^2}. \tag{12}$$

Nüüd eeldame, et k_i on reaalsed, ja arvutame läbilaskvuskoefitsiendi

$$\begin{aligned} |T_1|^2 &= \frac{1}{4} \left[L_1 \cos(\alpha) - i L_2 \sin(\alpha) \right] \left[L_1 \cos(\alpha) + i L_2 \sin(\alpha) \right] \\ &= \frac{1}{4} \left[L_1^2 \cos^2(\alpha) + L_2^2 \sin^2(\alpha) \right], \end{aligned} \tag{13}$$

$$\begin{aligned} T &= \frac{k_3}{k_1} \frac{1}{|T_1|^2} \\ &= \frac{k_3}{k_1} \frac{4}{L_1^2 \cos^2(\alpha) + L_2^2 \sin^2(\alpha)} \\ &= \frac{4}{\left(\sqrt{\frac{k_1}{k_3}} + \sqrt{\frac{k_3}{k_1}} \right)^2 \cos^2(\alpha) + \left(\frac{k_2}{\sqrt{k_1 k_3}} + \frac{\sqrt{k_1 k_3}}{k_2} \right)^2 \sin^2(\alpha)}. \end{aligned} \tag{14}$$

2. Kohaldage saadud valemid energiavahemikule $V_3 < E < V_2$.

Sellisel juhul on k_2 imaginaarne, defineerime $k_2 = i\kappa_2$, $\alpha' = \kappa_2 a$. Paneme tähele, et L_2 on puhtimaginaarne

$$L_2^* = \frac{-i\kappa_2}{k_1} + \frac{k_3}{-i\kappa_2} = -L_2. \tag{15}$$

Arvutame nüüd läbilaskvuskoefitsiendi:

$$\begin{aligned}
|4T_1|^2 &= [e^{\alpha'}(L_1+L_2)+e^{-\alpha'}(L_1-L_2)][e^{\alpha'}(L_1+L_2^*)+e^{-\alpha'}(L_1-L_2^*)] \\
&= [e^{\alpha'}(L_1+L_2)+e^{-\alpha'}(L_1-L_2)][e^{\alpha'}(L_1-L_2)+e^{-\alpha'}(L_1+L_2)] \\
&= e^{2\alpha'}(L_1^2-L_2^2)+(L_1+L_2)^2+(L_1-L_2)^2+e^{-2\alpha'}(L_1^2-L_2^2) \\
&= 2(L_1^2+L_2^2)+(e^{2\alpha'}+e^{-2\alpha'})(L_1^2-L_2^2) \\
&= 2(L_1^2+L_2^2)+2(\cosh^2(2\alpha'))(L_1^2-L_2^2) \\
&= 2(L_1^2+L_2^2)(-\sinh^2(\alpha')+\cosh^2(\alpha'))+2(\sinh^2(\alpha')+\cosh^2(\alpha'))(L_1^2-L_2^2) \\
&= 4(L_1^2\cosh^2(\alpha')-L_2^2\sinh^2(\alpha'))
\end{aligned} \tag{16}$$

$$\begin{aligned}
T &= \frac{k_3}{k_1}\frac{1}{|T_1|^2} \\
&= \frac{4}{\left(\sqrt{\frac{k_1}{k_3}}+\sqrt{\frac{k_3}{k_1}}\right)^2\cosh^2(\alpha')+\left(\frac{\kappa_2}{\sqrt{k_1k_3}}-\frac{\sqrt{k_1k_3}}{\kappa_2}\right)^2\sinh^2(\alpha')},
\end{aligned} \tag{17}$$

kus arvestasime, et $L_2^2=\left(\frac{i\kappa_2}{\sqrt{k_1k_3}}+\frac{\sqrt{k_1k_3}}{i\kappa_2}\right)^2=-\left(\frac{\kappa_2}{\sqrt{k_1k_3}}-\frac{\sqrt{k_1k_3}}{\kappa_2}\right)^2$.

3. Tõestage, et mistahes $E>V_1$ korral kehtib seos $R(E)+T(E)=1$.

1. **Juht $E>V_2$:**

   Analoogiliselt valemiga 13, saame:

$$|T_2|^2=\frac{1}{4}\left[L_3^2\cos^2(\alpha)+L_4^2\sin^2(\alpha)\right] \tag{18}$$

   ja

$$\begin{aligned}
R(E)+T(E) &= \frac{|T_2|^2+\frac{k_3}{k_1}}{|T_1|^2} \\
&= \frac{1}{4|T_1|^2}\left[(L_3^2+4\frac{k_3}{k_1})\cos^2(\alpha)+(L_4^2+4\frac{k_3}{k_1})\sin^2(\alpha)\right] \\
&= \frac{1}{4|T_1|^2}\left[L_1^2\cos^2(\alpha)+L_2^2\sin^2(\alpha)\right] \\
&= \frac{|T_1|^2}{|T_1|^2} \\
&= 1,
\end{aligned} \tag{19}$$

   kus arvestasime, et

$$\begin{aligned}
L_3^2+4\frac{k_3}{k_1} &= 1-2\frac{k_3}{k_1}+\frac{k_3^2}{k_1^2}+4\frac{k_3}{k_1}=L_1^2, \\
L_4^2+4\frac{k_3}{k_1} &= \frac{k_2^2}{k_1^2}-2\frac{k_3}{k_1}+\frac{k_3^2}{k_2^2}+4\frac{k_3}{k_1}=L_2^2.
\end{aligned} \tag{20}$$

2. **Juht $V_3<E<V_2$:**

Analoogiliselt valemiga 16 saame:

$$|T_2|^2 = \frac{1}{4}\left[L_3^2 \cosh^2(\alpha') - L_4^2 \sinh^2(\alpha')\right] \tag{21}$$

ja

$$\begin{aligned}
R(E) + T(E) &= \frac{|T_2|^2 + \frac{k_3}{k_1}}{|T_1|^2} \\
&= \frac{1}{4|T_1|^2}\left[(L_3^2 + 4\frac{k_3}{k_1}) \cosh^2(\alpha') - (L_4^2 + 4\frac{k_3}{k_1}) \sinh^2(\alpha')\right] \\
&= \frac{1}{4|T_1|^2}\left[L_1^2 \cosh^2(\alpha') - L_2^2 \sinh^2(\alpha')\right] \\
&= \frac{|T_1|^2}{|T_1|^2} \\
&= 1,
\end{aligned} \tag{22}$$

kus arvestasime valemeid 20.

3. **Juht $V_1 < E < V_3$:**

   $k_2^* = -k_2$, $k_3^* = -k_3$

$$\begin{aligned}
T_2^* &= \frac{1}{2}\left[\left(1 + \frac{k_3}{k_1}\right)\cos(-k_2 a) + \left(\frac{-k_2}{k_1} - \frac{k_3}{k_2}\right)\sin(-k_2 a)\right] \\
&= \frac{1}{2}\left[\left(1 + \frac{k_3}{k_1}\right)\cos(k_2 a) + \left(\frac{k_2}{k_1} + \frac{k_3}{k_2}\right)\sin(k_2 a)\right] \\
&= T_1.
\end{aligned} \tag{23}$$

Seega $|T_2|^2 = |T_1|^2$ ning $R(E) = 1$ ja sellest järelduvalt ka $T = 0$ (eeldades vihjes antud informatsiooni).

4. Tõestage, et kui $k_3 = k_1$, siis valem (2) on teisendatav kujule $T(E) = \left\{1 + \frac{\left[\sin\left(\sqrt{\frac{E-V}{C}}a\right)\right]^2}{4E/V(E/V-1)}\right\}^{-1}$

$$\frac{k_1^2}{k_1^2 - k_2^2} = \frac{E}{C\left(\frac{E}{C} - \frac{E-V}{C}\right)} = \frac{E}{V} \tag{24}$$

$$\frac{k_2^2}{k_1^2 - k_2^2} = \frac{E-V}{C\left(\frac{E}{C} - \frac{E-V}{C}\right)} = \frac{E}{V} - 1 \tag{25}$$

Ja valem 14 (ehk valem (2) juhendis) võtab kuju

$$
\begin{aligned}
T &= \frac{4}{\left(\sqrt{\frac{k_1}{k_1}}+\sqrt{\frac{k_1}{k_1}}\right)^2\cos^2(\alpha)+\left(\frac{k_2}{\sqrt{k_1k_1}}+\frac{\sqrt{k_1k_1}}{k_2}\right)^2\sin^2(\alpha)} \\
&= \frac{4}{4\cos^2(\alpha)+\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)^2\sin^2(\alpha)} \\
&= \frac{4}{4\cos^2(\alpha)+\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)^2\sin^2(\alpha)} \\
&= \left(\cos^2(\alpha)+\frac{1}{4}\left(\frac{k_2^2}{k_1^2}+2+\frac{k_1^2}{k_2^2}\right)\sin^2(\alpha)\right)^{-1} \\
&= \left(1+\frac{1}{4}\left(\frac{k_2^2}{k_1^2}-2+\frac{k_1^2}{k_2^2}\right)\sin^2(\alpha)\right)^{-1} \\
&= \left(1+\frac{1}{4}\left(\frac{k_2^2}{k_1^2}-2+\frac{k_1^2}{k_2^2}\right)\sin^2(\alpha)\right)^{-1} \\
&= \left(1+\frac{1}{4}\frac{1}{k_1^2k_2^2}\left(k_2^2-k_1^2\right)^2\sin^2(\alpha)\right)^{-1} \\
&= \left\{1+\frac{\left[\sin\left(\sqrt{\frac{E-V}{C}}a\right)\right]^2}{4E/V(E/V-1)}\right\}^{-1}
\end{aligned}
\tag{26}
$$

5. Tõestage, et joonisel kujutatud potentsiaalibarjääri läbilaskvus ei sõltu sellest, milline on pealelangeva laine suund: vasakult paremale (suund 1 $\rightarrow$ 3) või vastupidi - paremalt vasakule (suund 3 $\rightarrow$ 1). Piisab, kui analüüsite juhtumit $E > V_2$, kuid muidugi võite uurida ka juhtumit $E > V3$.

Ülekandemaatriks ja elemendi T_1' arvutused:

$$
T_{31} = \begin{bmatrix} T_1' & T_3' \\ T_2' & T_4' \end{bmatrix} = (T_{13})^{-1} = (D_{23})^{-1}(P_2)^{-1}(D_{12})^{-1} \tag{27}
$$

$$
\begin{aligned}
(D_{23})^{-1} &= \frac{2}{\left(1+\frac{k_3}{k_2}\right)^2-\left(1-\frac{k_3}{k_2}\right)^2}\begin{bmatrix} 1+\frac{k_3}{k_2} & \frac{k_3}{k_2}-1 \\ \frac{k_3}{k_2}-1 & 1+\frac{k_3}{k_2} \end{bmatrix} \\
&= \frac{k_2}{2k_3}\begin{bmatrix} 1+\frac{k_3}{k_2} & \frac{k_3}{k_2}-1 \\ \frac{k_3}{k_2}-1 & 1+\frac{k_3}{k_2} \end{bmatrix} \\
&= \frac{1}{2}\begin{bmatrix} 1+\frac{k_2}{k_3} & 1-\frac{k_2}{k_3} \\ 1-\frac{k_2}{k_3} & 1+\frac{k_2}{k_3} \end{bmatrix}
\end{aligned}
\tag{28}
$$

$$
(D_{12})^{-1} = \frac{1}{2}\begin{bmatrix} 1+\frac{k_1}{k_2} & 1-\frac{k_1}{k_2} \\ 1-\frac{k_1}{k_2} & 1+\frac{k_1}{k_2} \end{bmatrix} \tag{29}
$$

$$
\begin{aligned}
(P_2)^{-1} &= \frac{1}{e^{-ik_2a}e^{ik_2a}}\begin{bmatrix} e^{ik_2a} & 0 \\ 0 & e^{-ik_2a} \end{bmatrix} \\
&= \begin{bmatrix} e^{ik_2a} & 0 \\ 0 & e^{-ik_2a} \end{bmatrix}
\end{aligned} \tag{30}
$$

$$
(D_{23})^{-1}(P_2)^{-1} = \frac{1}{2}\begin{bmatrix} \left(1+\frac{k_2}{k_3}\right)e^{ik_2a} & \left(1-\frac{k_2}{k_3}\right)e^{-ik_2a} \\ \left(1-\frac{k_2}{k_3}\right)e^{ik_2a} & \left(1+\frac{k_2}{k_3}\right)e^{-ik_2a} \end{bmatrix} \tag{31}
$$

$$
\begin{aligned}
T_1' &= \frac{1}{4}\left[\left(1+\frac{k_2}{k_3}\right)\left(1+\frac{k_1}{k_2}\right)e^{ik_2a} + \left(1-\frac{k_2}{k_3}\right)\left(1-\frac{k_1}{k_2}\right)e^{-ik_2a}\right] \\
&= \frac{1}{4}\left[\left(1+\frac{k_1}{k_2}+\frac{k_2}{k_3}+\frac{k_1}{k_3}\right)e^{ik_2a} + \left(1-\frac{k_1}{k_2}-\frac{k_2}{k_3}+\frac{k_1}{k_3}\right)e^{-ik_2a}\right] \\
&= \frac{1}{2}\left[\left(1+\frac{k_1}{k_3}\right)\cos(k_2a) + i\left(\frac{k_1}{k_2}+\frac{k_2}{k_3}\right)\sin(k_2a)\right]
\end{aligned} \tag{32}
$$

Vaatleme juhtumit $E > V_2$:

$$
|T_1'|^2 = \frac{1}{4}\left[\left(1+\frac{k_1}{k_3}\right)^2\cos^2(k_2a) + \left(\frac{k_1}{k_2}+\frac{k_2}{k_3}\right)^2\sin^2(k_2a)\right] \tag{33}
$$

Läbilaskvuskoefitsient:

$$
T = \frac{|j_{1\leftarrow}|}{|j_{3\leftarrow}|} = \frac{k_1}{k_3|T_1'|^2} = \frac{4}{\left(\sqrt{\frac{k_3}{k_1}}+\sqrt{\frac{k_1}{k_3}}\right)^2\cos^2(k_2a) + \left(\frac{\sqrt{k_3k_1}}{k_2}+\frac{k_2}{\sqrt{k_1k_3}}\right)^2\sin^2(k_2a)}. \tag{34}
$$

Nagu näha, siis saadud tulemus langeb kokku valemiga 14.