

Theoretische Physik D - Quantenmechanik SS 2005

Übungsblatt 4 - Lösung

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Aufgabe 1

(i) Berechnung von Φ

$$\begin{aligned}\Psi_I(x) &= e^{ikx} + Ae^{-ikx} \\ \Psi_{II}(x) &= Be^{-\delta x} \\ k^2 &= \frac{2mE}{\hbar^2} \quad \delta^2 = \frac{2m}{\hbar^2}(V_0 - E)\end{aligned}$$

Anschlussbedingungen:

$$\Psi_I(0) = \Psi_{II}(0) \tag{1}$$

$$\Psi'_I(0) = \Psi'_{II}(0) \tag{2}$$

$$\text{aus (1) folgt:} \quad 1 + A = B$$

$$\text{aus (2) folgt:} \quad ik - ikA = -\delta B$$

$$\begin{aligned}ik(1 - A) &= -\delta(1 + A) \\ \Rightarrow A &= \frac{k - i\delta}{k + i\delta} = e^{-2i\alpha} \quad \alpha = \arctan \frac{\delta}{k}\end{aligned}$$

Umformung erfolgt mit den Hinweisen vom Übungsblatt 2, Aufgabe 2(i).

$$\begin{aligned}\Psi_R(x) &= e^{-2i\alpha} e^{-ikx} \\ \Rightarrow \quad \Phi &= \alpha = \arctan \frac{\delta}{k} = \underline{\underline{\arctan \sqrt{\left(\frac{2mV_0}{\hbar^2 k^2} - 1\right)}}}\end{aligned}$$

(ii) Berechnung von δt

$$\begin{aligned}
 \Psi(x, t) &= \int_0^\delta dk \, g(k) e^{i(kx - \omega t)} \\
 \omega &= \frac{E}{\hbar} = \frac{k^2 \hbar}{2m} \quad \delta' = \sqrt{\frac{2mV_0}{\hbar}} \\
 \Psi_R(x, t) &= \int_0^\delta dk \, g(k) e^{-i(kx + \omega t)} = \int_0^\delta dk \, e^{-i(kx + \omega t + 2\Phi)} \\
 x_M &= - \left. \frac{dx}{dk} \right|_{k=k_0} \quad \alpha = \omega t + 2\Phi \\
 x_M &= - \left. \frac{d\omega}{dk} t - 2 \frac{d\Phi}{dk} \right|_{k=k_0} \\
 - \left. \frac{d\omega}{dk} \right|_{k=k_0} &= - \frac{\hbar k_0}{m} \\
 \left. \frac{d\Phi}{dk} \right|_{k=k_0} &= \frac{d \arctan \sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1}}{dk} \\
 \left. \frac{d\Phi}{dk} \right|_{k=k_0} &= \frac{1}{1 + \left(\frac{2mV_0}{\hbar^2 k^2}\right) - 1} \cdot \frac{1}{2\sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1}} \cdot \frac{2mV_0}{\hbar^2} \cdot \frac{-2}{k^3} \\
 \left. \frac{d\Phi}{dk} \right|_{k=k_0} &= \frac{-1}{k\sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1}} \quad \Rightarrow \quad x_M = - \frac{\hbar k_0 t}{m} + \frac{2}{\sqrt{\frac{2mV_0}{\hbar^2} - k_0^2}}
 \end{aligned}$$

Es folgt ein Vergleich des quantenmechanischen Weges mit dem klassischen Weg $x_M = x_{KI}$.

$$\begin{aligned}
 x_{KI} &= v_0 t \quad v_0 = v = - \left. \frac{d\omega}{dk} \right|_{k=k_0} = - \frac{k_0 \hbar}{m} \\
 v_0 t_{KI} &= - \frac{\hbar k_0}{m} t_{QM} + \frac{2}{\sqrt{\frac{2mV_0}{\hbar^2} - k_0^2}} \\
 t_{QM} &= t_{KI} + \frac{2m}{\hbar k_0 \sqrt{\frac{2mV_0}{\hbar^2} - k_0^2}} = t_{KI} + \delta t
 \end{aligned}$$

Aufgabe 2

(i)

$$a_n = \frac{1}{\sqrt{\pi}} \left[\int_{-\pi}^0 dx f(x) \cos nx + \int_0^{+\pi} dx f(x) \cos nx \right]$$

Substituion: $x = -x' \quad dx = -dx'$

$$a_n = \frac{1}{\sqrt{\pi}} \left[- \int_{+\pi}^0 dx' f(-x') \cos -nx' + \int_0^{+\pi} dx f(x) \cos nx \right]$$

$$a_n = \frac{1}{\sqrt{\pi}} \left[\int_0^{+\pi} dx' f(-x') \cos nx' + \int_0^{+\pi} dx f(x) \cos nx \right]$$

$$a_n = \frac{1}{\sqrt{\pi}} \left[\int_0^{+\pi} dx' -f(x') \cos nx' + \int_0^{+\pi} dx f(x) \cos nx \right]$$

$$a_n = 0$$

$$b_n = \frac{1}{\sqrt{\pi}} \left[\int_{-\pi}^0 dx f(x) \sin nx + \int_0^{\pi} dx f(x) \sin nx \right]$$

Substituion: $x = -x' \quad dx = -dx'$

$$b_n = \frac{1}{\sqrt{\pi}} \left[- \int_{+\pi}^0 dx' f(-x') \sin -nx' + \int_0^{+\pi} dx f(x) \sin nx \right]$$

$$b_n = \frac{1}{\sqrt{\pi}} \left[\int_0^{+\pi} dx' f(x') - \sin nx' + \int_0^{+\pi} dx f(x) \sin nx \right]$$

$$b_n = 0$$

(ii)

$$f(x) = \begin{cases} -\sin x & -\pi \leq x \leq 0 \\ 0 & \text{ansonsten} \end{cases}$$

$$a_0 = -\frac{1}{\sqrt{2\pi}} \int_{-\pi}^0 dx \sin x = \frac{1}{\sqrt{2\pi}} \cos x \Big|_{-\pi}^0 = \sqrt{\frac{2}{\pi}}$$

Für $n \neq 1$ gilt für b_n :

$$\begin{aligned}
b_n &= \frac{1}{\sqrt{\pi}} \int_{-\pi}^0 dx (-1) \sin x \sin nx = \frac{1}{\sqrt{\pi}} \int_{-\pi}^0 dx (-1) \frac{e^{ix} - e^{-ix}}{2i} \cdot \frac{e^{inx} - e^{-inx}}{2i} \\
b_n &= \frac{1}{\sqrt{\pi}} \int_{-\pi}^0 dx \frac{1}{4} (e^{ix(1+n)} - e^{ix(1-n)} - e^{-ix(1-n)} + e^{-ix(1+n)}) \\
b_n &= \frac{1}{\sqrt{\pi}} \left[\frac{1}{4} \left(\frac{1}{(n+1)i} (e^{ix(1+n)} - e^{-ix(1+n)}) - \frac{1}{(1-n)i} (e^{ix(1-n)} - e^{-ix(1-n)}) \right) \right]_{-\pi}^0 \\
b_n &= \frac{1}{\sqrt{\pi}} \left[\frac{\sin(1+n)x}{2(1+n)} - \frac{\sin(1-n)x}{2(1-n)} \right]_{-\pi}^0 = 0
\end{aligned}$$

Für den Fall $n = 1$ ergibt sich b_1 :

$$b_1 = -\frac{1}{\sqrt{\pi}} \int_{-\pi}^0 dx \sin^2 x = -\frac{1}{\sqrt{\pi}} \underbrace{\left[\frac{1}{2}x - \frac{1}{4}\sin 2x \right]_{-\pi}^0}_{\text{Bronstein}} = -\frac{\pi}{2\sqrt{\pi}} = -\frac{\sqrt{\pi}}{2}$$

Analoge Vorgehensweise der Lösung des Integrals für a_n oder durch Bronstein:

$$\begin{aligned}
a_n &= -\frac{1}{\sqrt{\pi}} \int_0^{-\pi} dx \sin x \cos nx = -\frac{1}{\sqrt{\pi}} \underbrace{\left[-\frac{\cos(1+n)x}{2(1+n)} - \frac{\cos(1-n)x}{2(1-n)} \right]_{-\pi}^0}_{\text{Bronstein}} \\
a_n &= \begin{cases} \frac{1}{\sqrt{\pi}} \left(\frac{1}{1+n} + \frac{1}{1-n} \right) = \frac{1}{\sqrt{\pi}} \frac{2}{1-n^2} & n = 2m+1; m \in \mathbb{N} \\ 0 & \text{ansonsten} \end{cases}
\end{aligned}$$

(iii)

$$\begin{aligned}
f(x) &= \begin{cases} 1 & -\pi/2 < x < \pi/2 \\ 0 & \text{ansonsten} \end{cases} \\
a_0 &= \frac{1}{2\sqrt{\pi}} \int_{-\pi/2}^{\pi/2} dx = \sqrt{\frac{\pi}{2}} \quad \underbrace{b_n = 0}_{f(x) \text{ ist eine ungerade Funktion}}
\end{aligned}$$

$$a_n = \frac{1}{\sqrt{\pi}} \int_{-\pi/2}^{\pi/2} dx \cos nx = \frac{1}{\sqrt{\pi}} \left[\frac{\sin nx}{n} \right]_{-\pi/2}^{\pi/2}$$

$$a_n = \begin{cases} 0 & n = 2, 4, 6, \dots \\ \frac{2}{\sqrt{\pi n}} & n = 1, 5, 9, \dots \\ \frac{-2}{\sqrt{\pi n}} & n = 3, 7, 11, \dots \end{cases}$$

Aufgabe 3

(i)

Gegeben:

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}} |1\rangle + \frac{i}{2} |2\rangle + \frac{-i}{\sqrt{2}} |3\rangle$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{3}} |1\rangle + \frac{-i}{\sqrt{3}} |3\rangle$$

Gesucht ist $|\Psi_3\rangle$. Betrachtung von $|\Psi_2\rangle$ und der Bedingung $\langle\Psi_3|\Psi_2\rangle = 0$ führt zu (z.B.):

$$\langle\Psi_3| = \frac{-i}{\sqrt{3}} \langle 1| + \alpha \langle 2| + \frac{1}{\sqrt{3}} \langle 3|$$

Für die Bestimmung von α wird die zweite Bedingung $\langle\Psi_3|\Psi_1\rangle = 0$ überprüft. Daraus folgt:

$$\langle\Psi_3| = \frac{-i}{\sqrt{3}} \langle 1| + \frac{2\sqrt{2}}{\sqrt{3}} \langle 2| + \frac{1}{\sqrt{3}} \langle 3|$$

$$\Rightarrow |\Psi_3\rangle = \frac{i}{\sqrt{3}} |1\rangle + \frac{2\sqrt{2}}{\sqrt{3}} |2\rangle + \frac{1}{\sqrt{3}} |3\rangle$$

Normierung der Vektoren $|\Psi_1\rangle$, $|\Psi_2\rangle$ und $|\Psi_3\rangle$:

$$|\widehat{\Psi_1}\rangle = \frac{|\Psi_1\rangle}{\langle\Psi_1|\Psi_1\rangle} = \frac{|\Psi_1\rangle}{\sqrt{\frac{1}{2} + \frac{1}{4} + \frac{1}{2}}} = \frac{2}{\sqrt{5}} |\Psi_1\rangle$$

$$\begin{aligned}
|\widehat{\Psi}_2\rangle &= \frac{|\Psi_2\rangle}{\langle\Psi_2|\Psi_2\rangle} = \frac{|\Psi_2\rangle}{\sqrt{\frac{1}{3} + \frac{1}{3}}} = \frac{\sqrt{3}}{\sqrt{2}} |\Psi_2\rangle \\
|\widehat{\Psi}_3\rangle &= \frac{|\Psi_3\rangle}{\langle\Psi_3|\Psi_3\rangle} = \frac{|\Psi_3\rangle}{\sqrt{\frac{1}{3} + \frac{8}{3} + \frac{1}{3}}} = \frac{\sqrt{3}}{\sqrt{10}} |\Psi_3\rangle
\end{aligned}$$

$$\begin{aligned}
|\widehat{\Psi}_1\rangle &= \frac{1}{\sqrt{5}}(\sqrt{2}|1\rangle + i|2\rangle - \sqrt{2}i|3\rangle) \\
|\widehat{\Psi}_2\rangle &= \frac{1}{\sqrt{2}}(|1\rangle + i|3\rangle) \\
|\widehat{\Psi}_3\rangle &= \frac{1}{\sqrt{10}}(i|1\rangle + 2\sqrt{2}|2\rangle + |3\rangle)
\end{aligned}$$

(ii)

$$\begin{aligned}
P_{\Psi_1} &= |\Psi_1\rangle \langle\Psi_1| = \frac{1}{5}(\sqrt{2}, i, -\sqrt{2}i) \begin{pmatrix} \sqrt{2} \\ -i \\ \sqrt{2}i \end{pmatrix} \\
P_{\Psi_1} &= \frac{1}{5} \begin{pmatrix} 2 & \sqrt{2}i & -2i \\ -\sqrt{2}i & 1 & -\sqrt{2} \\ 2i & -\sqrt{2} & 2 \end{pmatrix} = P_{\Psi_1}^\dagger \Rightarrow \text{hermitesch!!} \\
P_{\Psi_2} &= |\Psi_2\rangle \langle\Psi_2| = \frac{1}{2}(1, 0, i) \begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix} \\
P_{\Psi_2} &= \frac{1}{2} \begin{pmatrix} 1 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 1 \end{pmatrix} = P_{\Psi_2}^\dagger \Rightarrow \text{hermitesch!!} \\
P_{\Psi_3} &= |\Psi_3\rangle \langle\Psi_3| = \frac{1}{10}(i, 2\sqrt{2}, 1) \begin{pmatrix} -i \\ 2\sqrt{2} \\ 1 \end{pmatrix} \\
P_{\Psi_3} &= \frac{1}{10} \begin{pmatrix} 1 & -2\sqrt{2}i & -i \\ 2\sqrt{2}i & 8 & 2\sqrt{2} \\ i & 2\sqrt{2} & 1 \end{pmatrix} = P_{\Psi_3}^\dagger \Rightarrow \text{hermitesch!!}
\end{aligned}$$

$$\sum_{i=1}^3 P_{\Psi_i} = \text{Einheitsmatrix} \Rightarrow \text{Vollständigkeit ist bewiesen.}$$

Aufgabe 4

(i)

$$\begin{aligned} L_y^\dagger = (L_y^*)^T &= -\frac{\hbar}{2i} \begin{pmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{\hbar}{2i} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} = L_y \Rightarrow \text{hermitesch!!} \end{aligned}$$

Bestimmung der Eigenwerte:

$$\begin{aligned} \text{Det}(L_y - \lambda \delta_{ij}) &= 0 \\ \begin{vmatrix} -\lambda & \sqrt{2}\frac{\hbar}{2i} & 0 \\ -\sqrt{2}\frac{\hbar}{2i} & -\lambda & \sqrt{2}\frac{\hbar}{2i} \\ 0 & -\sqrt{2}\frac{\hbar}{2i} & -\lambda \end{vmatrix} &= \underbrace{-\lambda \left(\lambda^2 - \hbar^2 \frac{1}{2} \right) - \sqrt{2}\frac{\hbar}{2i} \left(\sqrt{2}\frac{\hbar}{2i} \lambda - 0 \right)}_{\text{Entwicklung nach der ersten Zeile}} \\ &= -\lambda(\lambda^2 - \hbar^2) \\ \Rightarrow \lambda_1 &= 0 \quad \lambda_{2,3} = \pm \hbar \end{aligned}$$

Bestimmung der Eigenvektoren:

$$\underline{\underline{\lambda_1 = 0:}}$$

$$\begin{aligned} \begin{pmatrix} 0 & \frac{\hbar}{2i}\sqrt{2} & 0 \\ -\frac{\hbar}{2i}\sqrt{2} & 0 & \frac{\hbar}{2i}\sqrt{2} \\ 0 & -\frac{\hbar}{2i}\sqrt{2} & 0 \end{pmatrix} &\rightarrow \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} -1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &\Rightarrow \vec{e}_1 = \frac{1}{\sqrt{2}}(1, 0, 1)^T \end{aligned}$$

$$\underline{\underline{\lambda_1 = \hbar:}}$$

$$\begin{pmatrix} -\hbar & \frac{\hbar}{2i}\sqrt{2} & 0 \\ -\frac{\hbar}{2i}\sqrt{2} & -\hbar & \frac{\hbar}{2i}\sqrt{2} \\ 0 & -\frac{\hbar}{2i}\sqrt{2} & -\hbar \end{pmatrix} \rightarrow \begin{pmatrix} -2i & \sqrt{2} & 0 \\ -\sqrt{2} & -2i & \sqrt{2} \\ 0 & -\sqrt{2} & -2i \end{pmatrix} \rightarrow \begin{pmatrix} -2i & \sqrt{2} & 0 \\ -2i & 2\sqrt{2} & 2i \\ 0 & -\sqrt{2} & -2i \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} -2i & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 2i \\ 0 & -\sqrt{2} & -2i \end{pmatrix} \rightarrow \begin{pmatrix} -2i & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 2i \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & \frac{1}{\sqrt{2}}i & 0 \\ 0 & -\frac{1}{\sqrt{2}}i & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Rightarrow \vec{e}_2 = \frac{1}{2}(1, i\sqrt{2}, -1)^T$$

$\lambda_1 = -\hbar$:

$$\begin{pmatrix} \hbar & \frac{\hbar}{2i}\sqrt{2} & 0 \\ -\frac{\hbar}{2i}\sqrt{2} & \hbar & \frac{\hbar}{2i}\sqrt{2} \\ 0 & -\frac{\hbar}{2i}\sqrt{2} & \hbar \end{pmatrix} \rightarrow \begin{pmatrix} 2i & \sqrt{2} & 0 \\ -\sqrt{2} & 2i & \sqrt{2} \\ 0 & -\sqrt{2} & 2i \end{pmatrix} \rightarrow \begin{pmatrix} 2i & \sqrt{2} & 0 \\ 2i & 2\sqrt{2} & -2i \\ 0 & -\sqrt{2} & 2i \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} 2i & \sqrt{2} & 0 \\ 0 & \sqrt{2} & -2i \\ 0 & -\sqrt{2} & 2i \end{pmatrix} \rightarrow \begin{pmatrix} 2i & \sqrt{2} & 0 \\ 0 & \sqrt{2} & -2i \\ 0 & 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}}i & 0 \\ 0 & \frac{1}{\sqrt{2}}i & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Rightarrow \vec{e}_3 = \frac{1}{2}(1, -i\sqrt{2}, -1)^T$$

(ii)

Berechnung der Projektoren:

$$P_1 = \vec{e}_1 \vec{e}_1^\dagger = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} (1, 0, 1) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$P_2 = \vec{e}_2 \vec{e}_2^\dagger = \frac{1}{4} \begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} (1, -i\sqrt{2}, -1) = \frac{1}{4} \begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix}$$

$$P_3 = \vec{e}_3 \vec{e}_3^\dagger = \frac{1}{4} \begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix} (1, i\sqrt{2}, -1) = \frac{1}{4} \begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}$$

Vollständigkeit:

$$P_1 + P_2 + P_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Orthogonalität:

$$P_1 \cdot P_2 = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \frac{1}{4} \begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$P_2 \cdot P_3 = \frac{1}{4} \begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix} \frac{1}{4} \begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$P_1 \cdot P_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \frac{1}{4} \begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$