

Übung 1. Optical Theorem

See the proof and the discussion about the physical meaning in the section 6.4.1 of the script.

Übung 2. Scattering theory in 2D

- (a) In order to find the Green function, we need to solve the following equation (cf. Eq (6.4))

$$\left[\frac{\hbar^2}{2m} \nabla^2 + E \right] G(\mathbf{r}, E) = \delta^{(2)}(\mathbf{r}). \quad (\text{L.1})$$

We solve this differential equation by means of Fourier transformation (see Eq. (6.7))

$$\bar{G}(\mathbf{q}, E) = \int_{\mathbb{R}^2} d^2r e^{-i\mathbf{q}\mathbf{r}} G(\mathbf{r}, E), \quad G(\mathbf{r}, E) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} d^2q e^{i\mathbf{q}\mathbf{r}} \bar{G}(\mathbf{q}, E). \quad (\text{L.2})$$

The Fourier transform of Eq. (L.1) reads

$$\left(-\frac{\hbar^2 q^2}{2m} + E \right) \bar{G}(\mathbf{q}, E) = 1, \quad (\text{L.3})$$

and the solution is

$$\bar{G}(\mathbf{q}, E) = \frac{1}{E - \hbar^2 q^2 / 2m}. \quad (\text{L.4})$$

Hence

$$G(\mathbf{r}, E) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} d^2q \frac{e^{i\mathbf{q}\mathbf{r}}}{E - \hbar^2 q^2 / 2m} = -\frac{2m}{\hbar^2} \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} d^2q \frac{e^{i\mathbf{q}\mathbf{r}}}{q^2 - k^2}, \quad (\text{L.5})$$

where $k^2 = 2mE/\hbar^2$. The last integral can be calculated both in cartesian and polar coordinates. For the former way, the choice of q_x along \mathbf{r} (such that $\mathbf{q}\mathbf{r} = q_x r$) is very convenient. A detailed calculation for both cases is given in the section 3 of the reference¹. Here we do the calculation in polar coordinates following the above mentioned reference.

$$\begin{aligned} G(\mathbf{r}, E) &= -\frac{2m}{\hbar^2} \frac{1}{2\pi} \int_0^\infty dq \frac{q}{q^2 - k^2} \underbrace{\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{iqr \cos(\phi)}}_{\mathcal{J}_0(qr)} = -\frac{m}{\pi \hbar^2} \int_0^\infty dq \frac{q}{q^2 - k^2} \mathcal{J}_0(qr) \\ &= -\frac{m}{\pi \hbar^2} \int_0^\infty dq \frac{q}{q^2 - k^2} \underbrace{\frac{2}{\pi} \int_1^\infty du \frac{\sin(qru)}{\sqrt{u^2 - 1}}}_{\mathcal{J}_0(qr)} \end{aligned} \quad (\text{L.6})$$

$$= -\frac{2m}{\pi^2 \hbar^2} \int_1^\infty \frac{du}{\sqrt{u^2 - 1}} \int_0^\infty dq \frac{q \sin(qru)}{q^2 - k^2} = -\frac{2m}{\pi^2 \hbar^2} \int_1^\infty \frac{du S(u)}{\sqrt{u^2 - 1}}. \quad (\text{L.7})$$

Above we used two integral representations of $\mathcal{J}_0(x)$ given in the exercise sheet. Now we need to calculate $S(u)$ given by

$$S(u) = \int_0^\infty dq \frac{q \sin(qru)}{q^2 - k^2} = \frac{1}{4i} \left(\int_{-\infty}^\infty dq \frac{q e^{iqr u}}{q^2 - k^2} - \int_{-\infty}^\infty dq \frac{q e^{-iqr u}}{q^2 - k^2} \right) = \frac{1}{4i} [E_+(u) - E_-(u)].$$

¹Revista Brasileira de Ensino de Física, v. 35, n. 1, 1304 (2013), <http://www.sbfisica.org.br/rbef/pdf/351304.pdf>

The last integrals have exactly the same form as the integral in the Eq. (6.9) of the script. These integrals mathematically are ill-defined. The integrand function has poles on the real axis $q = \pm k$. We can use the residue theorem and the prescription of circumventing the poles (see the discussion after Eq. (6.9) in the script). We need to decide how to choose the contour in the q -plane in order to get the Green function with right boundary conditions (Causality implies we should have outgoing waves from the point source at $\mathbf{r} = 0$). For the first integral we must close the contour with infinite semicircle in the upper half-plane, and for the second integral in the lower half-plane. In this way, according to Jordan's lemma, the semicircle at infinity would contribute nothing. Depending on how we circumvent the poles on the real axis, the result will be different (ref. 1 gives all the possible results). We choose the contours as shown in Fig. 1.

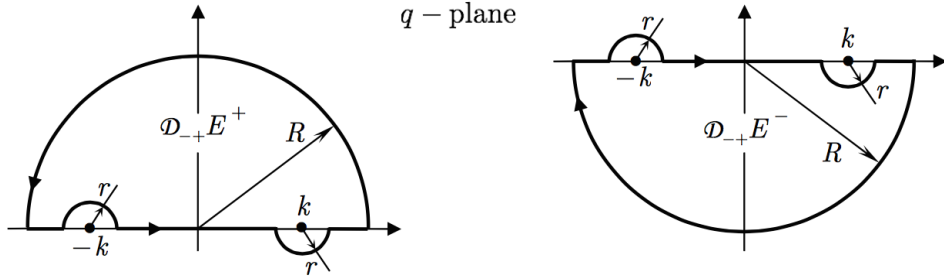


Abbildung 1: The integration contours in q -plane to calculate the integrals $E_+(u)$ and $E_-(u)$.

For this choice

$$S(u) = \frac{1}{4i} 2\pi i \left[\text{Res}\left(\frac{qe^{iqu}}{q^2 - k^2}, k\right) + \text{Res}\left(\frac{qe^{-iqu}}{q^2 - k^2}, -k\right) \right] = \frac{\pi}{2} (e^{ikru}/2 + e^{ikru}/2) = \frac{\pi}{2} e^{ikru}. \quad (\text{L.8})$$

Hence

$$G(\mathbf{r}, E) = -\frac{m}{\pi\hbar^2} \int_1^\infty du \frac{e^{ikru}}{\sqrt{u^2 - 1}} = -i \frac{m}{2\hbar^2} \mathcal{H}_0^{(1)}(kr). \quad (\text{L.9})$$

Above we have used the integral representation of the first Hankel function given in the exercise sheet.

- (b) Similar to Eq. (6.12) the solution of the scattering problem is given by Lippmann-Schwinger equation

$$\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} + \int d^2r' G(\mathbf{r} - \mathbf{r}', E_k) V(\mathbf{r}') \Psi_{\mathbf{k}}(\mathbf{r}'). \quad (\text{L.10})$$

At large distances $r \rightarrow \infty$, $k|\mathbf{r} - \mathbf{r}'| \approx kr - k\hat{\mathbf{r}}\mathbf{r}'$, ($\hat{\mathbf{r}} = \mathbf{r}/r$) and

$$G(\mathbf{r} - \mathbf{r}', E_k) \sim -i \frac{m}{2\hbar^2} \sqrt{\frac{2}{\pi kr}} e^{i(kr - k\hat{\mathbf{r}}\mathbf{r}' - \pi/4)}. \quad (\text{L.11})$$

We have used that for large $x \gg 1$ the first Hankel function of the l -th order has the following asymptotic form

$$\mathcal{H}_l^{(1)}(x) \sim \sqrt{\frac{2}{\pi x}} e^{i(x - \pi/4 - l\pi/2)}, \quad (\text{L.12})$$

and $1/\sqrt{|\mathbf{r} - \mathbf{r}'|} \approx 1/\sqrt{r}$. Hence for large r

$$\Psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\mathbf{r}} + f_k(\varphi) \frac{e^{ikr}}{\sqrt{r}}, \quad (\text{L.13})$$

where

$$f_k(\varphi) = -i \frac{m}{2\hbar^2} \sqrt{\frac{2}{\pi k}} e^{-i\pi/4} \int d^2 r' e^{-ik\hat{r}r'} V(\mathbf{r}') \Psi_{\mathbf{k}}(\mathbf{r}'). \quad (\text{L.14})$$

In the similar way as in the 3D case, one can express the total cross section and differential cross section by $f_k(\varphi)$ (see Eq. (6.15) and Eq. (6.16)).

(c) We want to solve the following equation for $\Psi_{\mathbf{k}}(\mathbf{r})$

$$\left[\frac{\hbar^2}{2m} \underbrace{\left(\partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_\varphi^2 \right)}_{\Delta_{2D}} + E_k \right] \Psi_{\mathbf{k}}(r, \varphi) = V(r) \Psi_{\mathbf{k}}(r, \varphi) \quad (\text{L.15})$$

In the case of centrally symmetric potential $V(r)$ we can separate the angular part and the radial part by using the ansatz given in the exercise sheet. The equation for the radial part $R_l(r)$ reads

$$\left(\partial_r^2 + \frac{1}{r} \partial_r - \frac{l^2}{r^2} + k^2 \right) R_l(r) = \frac{2m}{\hbar^2} V(r) R_l(r). \quad (\text{L.16})$$

If $V \equiv 0$, Eq. (L.16) is the Bessel equation and the physical solution is $R_l(r) = \mathcal{J}_l(r)$ (cf. exercise 3 of the series 9).

$$V \equiv 0 \quad R_l(r) = \mathcal{J}_l(r) = \frac{1}{2} \left[\mathcal{H}_l^{(2)} + \mathcal{H}_l^{(1)} \right]. \quad (\text{L.17})$$

(d) If $V \neq 0$, in analogy with (6.42), we write down the asymptotic radial wavefunction as

$$R_l(r) \sim \alpha_l \left[\mathcal{H}_l^{(2)} + s_l \mathcal{H}_l^{(1)} \right]. \quad (\text{L.18})$$

Due to particle number conservation (which only holds for an elastic scattering) it follows that $|s_l| = 1$. Like in the 3D case we denote $s_l = e^{2i\delta_l(k)}$ (cf. Eq. (6.46)). The overall phase α_l will be fixed later. Similar to Eq. (6.40), plane waves in 2D can be expressed as a superposition of solutions of the case of $V \equiv 0$:

$$e^{i\mathbf{k}\mathbf{r}} = e^{ikr \cos \varphi} = \sum_{l=-\infty}^{\infty} \mathcal{J}_l(kr) e^{il\pi/2} e^{il\varphi} = \frac{1}{2} \sum_{l=-\infty}^{\infty} \left[\mathcal{H}_l^{(1)}(kr) + \mathcal{H}_l^{(2)}(kr) \right] e^{il\pi/2} e^{il\varphi}. \quad (\text{L.19})$$

Hence the total wavefunction of the scattering state can be written as

$$\begin{aligned} \Psi_{\mathbf{k}}(\mathbf{r}) &= \sum_{l=-\infty}^{\infty} R_l(r) e^{il\varphi} \sim \sum_{l=-\infty}^{\infty} \alpha_l \left[\mathcal{H}_l^{(2)}(kr) + e^{2i\delta_l(k)} \mathcal{H}_l^{(1)}(kr) \right] e^{il\varphi} \\ &= e^{i\mathbf{k}\mathbf{r}} + \sum_{l=-\infty}^{\infty} \left\{ \left[\alpha_l - \frac{1}{2} e^{il\pi/2} \right] \mathcal{H}_l^{(2)}(kr) + \left[\alpha_l e^{2i\delta_l(k)} - \frac{1}{2} e^{il\pi/2} \right] \mathcal{H}_l^{(1)}(kr) \right\} e^{il\varphi} \end{aligned} \quad (\text{L.20})$$

Since we want to have only plane wave and outgoing waves we have to fix α_l such that the coefficient of $\mathcal{H}_l^{(2)}(kr)$ vanishes. Hence we fix $\alpha_l = \frac{1}{2} e^{il\pi/2}$, and the total wavefunction takes the following form:

$$\Psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\mathbf{r}} + \frac{1}{2} \sum_{l=-\infty}^{\infty} (e^{2i\delta_l(k)} - 1) \mathcal{H}_l^{(1)}(kr) e^{il\pi/2} e^{il\varphi} \quad (\text{L.21})$$

(e) At large distances we can use (L.12) and write the wavefunction in the form of (L.13)

$$\Psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\mathbf{r}} + \left[\sqrt{\frac{1}{2\pi k}} e^{-i\pi/4} \sum_{l=-\infty}^{\infty} (e^{2i\delta_l} - 1) e^{il\varphi} \right] \frac{e^{ikr}}{\sqrt{r}}. \quad (\text{L.22})$$

Hence

$$f_k(\varphi) = \sqrt{\frac{1}{2\pi k}} e^{-i\pi/4} \sum_{l=-\infty}^{\infty} (e^{2i\delta_l} - 1) e^{il\varphi} = \sqrt{\frac{2}{\pi k}} e^{i\pi/4} \sum_{l=-\infty}^{\infty} e^{i\delta_l} \sin(\delta_l) e^{il\varphi}. \quad (\text{L.23})$$

Using the last result one can calculate the total scattering cross section

$$\sigma = \int_{-\pi}^{\pi} d\varphi |f_k(\varphi)|^2 = \frac{2}{\pi k} \sum_{l,l'} e^{i(\delta_l - \delta_{l'})} \sin(\delta_l) \sin(\delta_{l'}) \int_{-\pi}^{\pi} d\varphi e^{i(l-l')\varphi} \quad (\text{L.24})$$

$$= \frac{2}{\pi k} 2\pi \sum_{l,l'} e^{i(\delta_l - \delta_{l'})} \sin(\delta_l) \sin(\delta_{l'}) \delta_{ll'} = \frac{4}{k} \sum_{l=-\infty}^{\infty} \sin^2(\delta_l). \quad (\text{L.25})$$

We note that

$$\text{Im}[f_k(0)e^{-i\pi/4}] = \sqrt{\frac{2}{\pi k}} \sum_{l=-\infty}^{\infty} \sin^2(\delta_l). \quad (\text{L.26})$$

Hence

$$\sigma = \sqrt{\frac{8\pi}{k}} \text{Im}[f_k(0)e^{-i\pi/4}]. \quad (\text{L.27})$$

The last equation is the optical theorem in the case of 2D scattering.

Übung 3. Dekohärenz eines Qubits

(a) Für einen reinen Zustand berechnen wir $\rho = |\psi\rangle\langle\psi|$ und finden

$$\rho_{\text{rein}} = |\alpha|^2 |0\rangle\langle 0| + \alpha\beta^* |0\rangle\langle 1| + \alpha^*\beta |1\rangle\langle 0| + |\beta|^2 |1\rangle\langle 1| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}. \quad (\text{L.28})$$

Ein gemischter Zustand in dem man sich mit Wahrscheinlichkeit $|\alpha|^2$ in $|0\rangle$ befindet und mit Wahrscheinlichkeit $|\beta|^2$ in $|1\rangle$, ist gegeben durch:

$$\rho_{\text{gemischt}} = |\alpha|^2 |0\rangle\langle 0| + |\beta|^2 |1\rangle\langle 1| = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}. \quad (\text{L.29})$$

In beide Fälle muss gelten dass $|\alpha|^2 + |\beta|^2 = 1$, so dass $\text{Tr}\rho = 1$ und wir einen korrekt normierten Zustand beschreiben. Der unterschied ist allerdings dass die off-diagonale eintritte in ρ (auch die kohärenzen genannt) in den gemischten Zustand verschwinden. Zum Schluss berechnen wir noch:

$$\text{Tr}\rho_{\text{rein}}^2 = \text{Tr} \begin{pmatrix} |\alpha|^4 + |\alpha|^2|\beta|^2 & \alpha\beta^*(|\alpha|^2 + |\beta|^2) \\ \alpha^*\beta(|\alpha|^2 + |\beta|^2) & |\beta|^4 + |\alpha|^2|\beta|^2 \end{pmatrix} \quad (\text{L.30})$$

$$= |\alpha|^4 + 2|\alpha|^2|\beta|^2 + |\beta|^4 = (|\alpha|^2 + |\beta|^2)^2 = 1, \quad (\text{L.31})$$

und

$$\text{Tr}\rho_{\text{gemischt}}^2 = \text{Tr} \begin{pmatrix} |\alpha|^4 & 0 \\ 0 & |\beta|^4 \end{pmatrix} = |\alpha|^4 + |\beta|^4 \leq 1. \quad (\text{L.32})$$

In Gl. (L.32) is $\text{Tr}\rho_{\text{gemischt}}$ nur gleich 1 wenn entweder $\alpha = 1$ und $\beta = 0$ oder umgekehrt. Aber in die Fälle beschreiben wir tatsächlich die reine Zustände $|\psi\rangle = |0\rangle$ und $|\psi\rangle = |1\rangle$.

(b) Die Dichte-Matrix für unser Qubit sieht nun so aus:

$$\rho(\phi) = \begin{pmatrix} |\alpha|^2 & \alpha\beta^*e^{-i\phi} \\ \alpha^*\beta e^{i\phi} & |\beta|^2 \end{pmatrix} = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}, \quad (\text{L.33})$$

wobei wir in den Zweite Linie ρ_{ij} eingeführt haben als vereinfachung der Notation. Wir rechnen nun das Integral separat für die eintritte ρ_{ij} der Dichte-Matrix aus. Zuerst betrachten wir die Diagonal-Elemente:

$$\rho_{00}(t) = \int d\phi P(\phi)\rho_{00}(\phi) = |\alpha|^2 \int d\phi P(\phi, t) = |\alpha|^2, \quad (\text{L.34})$$

weil $P(\phi, t)$ ein normierte Gausssche-verteilung ist. Ebenso finden wir $\rho_{11}(t) = |\beta|^2$, und finden damit dass die Diagonal-Elemente der Dichte-Matrix zeit-unabhängig sind. Für ρ_{01} finden wir:

$$\rho_{01}(t) = \int d\phi P(\phi)\rho_{01}(\phi) = \alpha\beta^* \frac{1}{\sqrt{2\pi\sigma(t)}} \int d\phi e^{-\frac{\tau}{4t}\phi^2 - i\phi} \quad (\text{L.35})$$

$$= \alpha\beta^* \frac{1}{\sqrt{2\pi\sigma(t)}} \sqrt{\frac{4\pi t}{\tau}} e^{-t/\tau} = \alpha\beta^* e^{-t/\tau}. \quad (\text{L.36})$$

Wegen hermitizität von ρ wissen wir auch direkt $\rho_{10} = \rho_{01}^* = \alpha^*\beta e^{-t/\tau}$. Die Off-Diagonale eintritte von ρ zerfallen also mit der Zeit, und unser Qubit geht von reiner Zustand zu einen gemischten Zustand. Die Konstante τ kann also als Dekohärenz-Zeit interpretiert werden.

(c) Wir berechnen die Eigenwerten von $\rho(t)$ am einfachsten in dem wir $\rho(t)$ zuerst zerlegen als $\rho(t) = \frac{1}{2}\hat{1} + \mathbf{b} \cdot \boldsymbol{\sigma}$, wobei $\boldsymbol{\sigma}$ einen Vektor aus die Pauli-Matrizen $\{\sigma_x, \sigma_y, \sigma_z\}$ ist. Wir wissen dann direkt dass die Eigenwerten gegeben sind durch:

$$\epsilon_1 = \frac{1}{2} + |b| \quad \text{und} \quad \epsilon_2 = \frac{1}{2} - |b|.$$

Die Entropie lässt sich dann berechnen via

$$S(t) = -\epsilon_1 \ln \epsilon_1 - \epsilon_2 \ln \epsilon_2.$$

Wir finden hier für \mathbf{b} :

$$\mathbf{b} = \frac{1}{2} \left\{ (\alpha\beta^* + \alpha^*\beta)e^{-t/\tau}, i(\alpha\beta^* - \alpha^*\beta)e^{-t/\tau}, |\alpha|^2 - |\beta|^2 \right\}, \quad (\text{L.37})$$

und damit:

$$|b| = \frac{1}{2} \sqrt{|\alpha|^4 + |\beta|^4 - 2|\alpha|^2|\beta|^2(1 - 2e^{-2t/\tau})} \quad (\text{L.38})$$

Für $\alpha = \beta = 1/\sqrt{2}$ lässt sich $|b|$ vereinfachen zu:

$$|b| = \frac{1}{2} e^{-t/\tau}, \quad (\text{L.39})$$

und damit ist die Entropie:

$$S(t) = - \left(\frac{1}{2} + \frac{1}{2} e^{-t/\tau} \right) \ln \left(\frac{1}{2} + \frac{1}{2} e^{-t/\tau} \right) - \left(\frac{1}{2} - \frac{1}{2} e^{-t/\tau} \right) \ln \left(\frac{1}{2} - \frac{1}{2} e^{-t/\tau} \right) \quad (\text{L.40})$$

Wir sehen dass $\lim_{t \rightarrow 0} S(t) = 0$, und $\lim_{t \rightarrow \infty} S(t) = \ln(2)$. Diese beide Werten reflektieren dass wir am Anfang sehr präzise wissen wie unser Zustand aussieht, aber im $t \rightarrow \infty$ Limes haben wir nur noch eine statistische Mischung aus 50% $|0\rangle$ und 50% $|1\rangle$.