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# GREEN's Function of the HELMHOLTZ Equation

## Calculation in Position Space

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# Abstract

In these notes, we present some details on the calculation of

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) \coloneqq \frac{\hbar^2}{2m}\,\langle\boldsymbol{x}\big|(E-\hat{H}_0\pm\mathrm{i}\epsilon)^{-1}\big|\boldsymbol{x'}\rangle$$
$$= -\frac{1}{4\pi}\frac{\mathrm{e}^{\pm\mathrm{i}k|\boldsymbol{x}-\boldsymbol{x'}|}}{|\boldsymbol{x}-\boldsymbol{x'}|}$$

performed in the lecture, which represents a so-called propagator in position space and appeared in the context of the Lippmann–Schwinger equation. Here, the energy is given by $E = \hbar^2k^2/(2m)$, with $k = |\boldsymbol{k}|$. We will not prove that this function indeed is the Green's function of the Helmholtz equation, *i.e.*, that it fulfills

$$(\nabla^2 + k^2)G_\pm(\boldsymbol{x},\boldsymbol{x'}) = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x'}),$$

which is part of this term's exercise sheets. In order to keep the actual calculation as clear and comprehensible as possible, we proceed in two steps: we first state and prove three minor theorems from complex analysis and then, making use of the last of these theorems, proceed with the aforementioned calculation in the main part of our notes. The ideas presented in our notes are based on Refs. [1–5] and we refrain from repeatedly citing these. For more details and rigorous proofs of the theorems presented here, the interested reader is referred to the above references and his or her favorite book on complex analysis.

# 1. Theorems

In this section, we prove the so-called Estimation Lemma/ML Inequality [4] and two propositions [3] that can be deduced from it. The latter of these propositions will be used for the calculation of the HELMHOLTZ equation's GREEN's function in the main part of our notes. Note that our proofs lack mathematical rigor for the sake of comprehensibility; the reader who wants to see a more rigorous proof should be able to do so in his or her favorite book on complex analysis.

**Lemma 1** (Estimation Lemma/ML Inequality). *Let $f(z)\colon \Omega \to \mathbb{C}$ be a complex-valued, continuous function on $\Omega \subseteq \mathbb{C}$ and $\gamma\colon [t_i, t_f] \to \Omega$ a curve parameterized by the interval $[t_i, t_f] \subseteq \mathbb{R}$. If $|f(z)|$ is bounded on $\gamma$, i.e., $M \coloneqq \sup_{z\in\gamma}|f(z)| < \infty$ exists, then*

$$\left| \int_\gamma \mathrm{d}z\, f(z) \right| \leq ML(\gamma),$$

*where*

$$L(\gamma) \coloneqq \int_{t_i}^{t_f} \mathrm{d}t\, |\gamma'(t)|$$

*is the arc length of the curve.*

*Proof.* We insert the definition of the complex contour integral by means of the parameterization of the curve $\gamma$ and use the triangle inequality for complex integrals to find

$$\begin{aligned} \left| \int_\gamma \mathrm{d}z\, f(z) \right| &= \left| \int_{t_i}^{t_f} \mathrm{d}t\, f(\gamma(t))\gamma'(t) \right| \\ &\leq \int_{t_i}^{t_f} \mathrm{d}t\, |f(\gamma(t))||\gamma'(t)|. \end{aligned}$$

Since, by assumption, $M = \sup_{z\in\gamma}|f(z)|$ exists and represents a constant upper bound for the function's absolute value on $\gamma$, $|f(z)| \leq M$ for $z \in \gamma$, we have

$$\left| \int_\gamma \mathrm{d}z\, f(z) \right| \leq M \int_{t_i}^{t_f} \mathrm{d}t\, |\gamma'(t)| = ML(\gamma),$$

where we used the definition of the length of the curve, $L(\gamma)$. □

**Proposition 2.** *Let $f_\pm(z)\colon \mathbb{R} \to \mathbb{C}$ be a complex-valued, continuous function that can be analytically continued into the upper ($f_+(z)$) or lower ($f_-(z)$) complex half-plane $\mathbb{H}_\pm \coloneqq \{z \in \mathbb{C} : \pm\mathrm{Im} z > 0\}$ except for a countable set of poles $\{a_1, \ldots, a_n\} \in \mathbb{C}$, i.e., $f_\pm(z)\colon \mathbb{H}_\pm \setminus \{a_1, \ldots, a_n\} \to \mathbb{C}$ (and, by analytic continuation, is also continuous there). In particular, we further assume that $f_\pm(z)$ can be written as the quotient of*

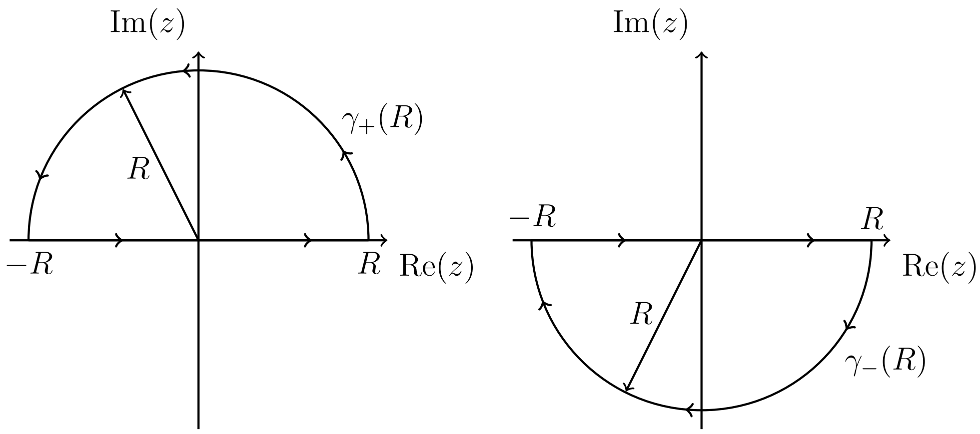


Figure 1: The integration contours $\Gamma_\pm(R) = [-R, R] \cup \gamma_\pm(R)$ in the complex plane, given by a straight line of length $2R$ on the $x$-axis and an upper/lower arc of radius $R$.

*two polynomials $p(z)$ and $q(z)$,*

$$f_\pm(z) = \frac{p(z)}{q(z)},$$

*with deg$(p) \leq$ deg$(q) - 2$ and $q(z)$ has no real zeroes, i.e., $q(z) \neq 0$ for $z \in \mathbb{R}$. Then,*

$$\int_{-\infty}^{\infty} \mathrm{d}z\, f_\pm(z) = \lim_{R\to\infty} \oint_{\Gamma_\pm(R)} \mathrm{d}z\, f_\pm(z),$$

*where $\Gamma_\pm(R)$ are the closed contours depicted in Fig. 1.*

*Proof.* Since, by assumption, $p(z)$ and $q(z)$ are polynomials, we have

$$p(z) = \sum_{i=0}^{\deg(p)} \alpha_i z^i, \qquad\qquad q(z) = \sum_{i=0}^{\deg(q)} \beta_i z^i.$$

Using the (reverse) triangle inequality, we obtain

$$|p(z)| \leq |\alpha_{\deg(p)}||z|^{\deg(p)} + \left| \sum_{i=0}^{\deg(p)-1} \alpha_i z^i \right| = |z|^{\deg(p)} \left( |\alpha_{\deg(p)}| + \left| \sum_{i=0}^{\deg(p)-1} \alpha_i \frac{z^i}{z^{\deg(p)}} \right| \right),$$

$$|q(z)| \geq \left| |\beta_{\deg(q)}||z|^{\deg(q)} - \left| \sum_{i=0}^{\deg(q)-1} \beta_i z^i \right| \right| = |z|^{\deg(q)} \left| |\beta_{\deg(q)}| - \left| \sum_{i=0}^{\deg(q)-1} \beta_i \frac{z^i}{z^{\deg(q)}} \right| \right|,$$

where

$$\left| \sum_{i=0}^{\deg(r)-1} \rho_i \frac{z^i}{z^{\deg(r)}} \right| \leq \sum_{i=0}^{\deg(r)-1} |\rho_i| \left| \frac{z^i}{z^{\deg(r)}} \right| \overset{|z|\to\infty}{\longrightarrow} 0$$

for both $r(z) \in \{p(z), q(z)\}$, $\rho_i \in \{\alpha_i, \beta_i\}$. Hence, by definition, for all $\varepsilon > 0$, there exists $B > 0$ such that

$$\Big| \sum_{i=0}^{\deg(r)-1} \rho_i \frac{z^i}{z^{\deg(r)}} \Big| < \varepsilon$$

for $|z| > B$, *e.g.*, $\varepsilon = |\rho_{\deg(r)}|/2$. In other words, there exist constants $c_p, c_q \in \mathbb{R}$ such that $|p(z)| \leq c_p |z|^{\deg(p)}$ and $|q(z)| \geq c_q |z|^{\deg(q)}$ for sufficiently large $|z|$. Consequently,

$$\left| \frac{p(z)}{q(z)} \right| \leq \frac{c_p |z|^{\deg(p)}}{c_q |z|^{\deg(q)}} \leq \frac{c}{|z|^2}$$

for $c := c_p / c_q \in \mathbb{R}$ and large enough $|z|$ due to the assumption $\deg(p) \leq \deg(q) - 2$.

In order to prove the proposition,

$$\int_{-\infty}^{\infty} \mathrm{d}z \, \frac{p(z)}{q(z)} = \lim_{R\to\infty} \oint_{\Gamma_\pm(R)} \mathrm{d}z \, \frac{p(z)}{q(z)},$$

we will show that

$$\lim_{R\to\infty} \int_{\gamma_\pm(R)} \mathrm{d}z \, \frac{p(z)}{q(z)} = 0,$$

where $\gamma_\pm(R)$ are the arcs depicted in Fig. 1. To this end, we parameterize the integration contour by means of

$$\gamma_\pm(R) \colon z = R\mathrm{e}^{\pm \mathrm{i}\varphi},$$

where $\varphi \in [0, \pi]$, so that $|z| = \mathrm{R}$. Assuming $R$ large and using Lemma 1 with

$$M_{\gamma_\pm(R)} = \sup_{z\in\gamma_\pm(R)} \left| \frac{p(z)}{q(z)} \right| \leq \sup_{z\in\gamma_\pm(R)} \frac{c}{|z|^2} = \frac{c}{R^2}$$

and $L(\gamma_\pm(R)) = \pi R$, we thus obtain

$$\left| \int_{\gamma_\pm(R)} \mathrm{d}z \, \frac{p(z)}{q(z)} \right| \leq M_{\gamma_\pm(R)} L(\gamma_\pm(R)) \leq \frac{\pi c}{R} \overset{R\to\infty}{\to} 0.$$

Since the integral vanishes if its absolute value does, this completes the proof. □

*Remark in advance:* the assumptions of the second proposition are very similar to the assumptions of the first one. However, instead of assuming that $f(z)$ is merely given by the quotient of two polynomials, we additionally multiply it with an exponential function here. As a result, the condition imposed on the degrees of the polynomials can be relaxed a bit but, at the same time, the analytic continuation into the upper/lower complex half-plane depends on the sign in the exponential.

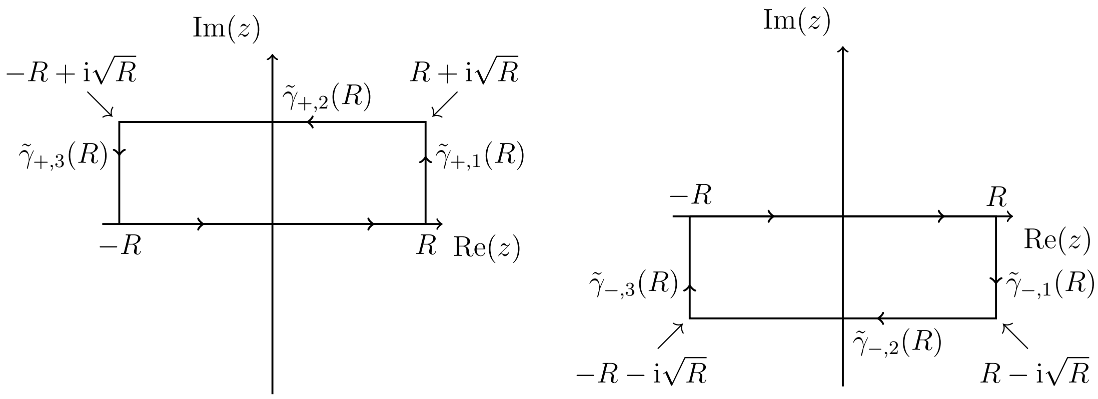


Figure 2: The closed integration contours $\tilde{\Gamma}_{\pm}(R) = [-R, R] \cup \tilde{\gamma}_{\pm,1}(R) \cup \tilde{\gamma}_{\pm,2}(R) \cup \tilde{\gamma}_{\pm,3}(R)$ in the complex plane, given by a straight line of length $2R$, which is completed to an upper/lower rectangle with height $\sqrt{R}$.

**Proposition 3.** *Let $g_{\pm}(z)\colon \mathbb{R} \to \mathbb{C}$ be a complex-valued, continuous function that can be analytically continued into the upper ($g_+(z)$) or lower ($g_-(z)$) complex half-plane $\mathbb{H}_{\pm} := \{z \in \mathbb{C} : \pm \mathrm{Im} z > 0\}$ except for a countable set of poles $\{a_1, \dots, a_n\} \in \mathbb{C}$, i.e., $g_{\pm}(z)\colon \mathbb{H}_{\pm} \setminus \{a_1, \dots, a_n\} \to \mathbb{C}$ (and, by analytic continuation, is also continuous there). In particular, we further assume that $g_{\pm}(z)$ is of the form*

$$g_{\pm}(z) = \frac{P(z)}{Q(z)} \mathrm{e}^{\pm \mathrm{i}\alpha z},$$

*where $P(z)$ and $Q(z)$ are two polynomials with deg$(P) \leq$ deg$(Q) - 1$, $\alpha > 0$, and $Q(z)$ has no real zeroes, i.e., $Q(z) \neq 0$ for $z \in \mathbb{R}$. Then,*

$$\int_{-\infty}^{\infty} \mathrm{d}z\, g_{\pm}(z) = \lim_{R \to \infty} \oint_{\tilde{\Gamma}_{\pm}(R)} \mathrm{d}z\, g_{\pm}(z),$$

*where $\tilde{\Gamma}_{\pm}(R)$ are the closed contours depicted in Fig. 2.*

*Proof.* Similar to the proof of Proposition 2, we can find a constant $C \in \mathbb{R}$ such that

$$\left| \frac{P(z)}{Q(z)} \right| \leq \frac{C}{|z|}$$

for large $|z|$ due to the assumption $\deg(P) \leq \deg(Q) - 1$. In order to prove

$$\int_{-\infty}^{\infty} \mathrm{d}z\, \frac{P(z)}{Q(z)} \mathrm{e}^{\pm \mathrm{i}\alpha z} = \lim_{R \to \infty} \oint_{\tilde{\Gamma}_{\pm}(R)} \mathrm{d}z\, \frac{P(z)}{Q(z)} \mathrm{e}^{\pm \mathrm{i}\alpha z},$$

we will show that

$$\lim_{R \to \infty} \int_{\tilde{\gamma}_{\pm,i}(R)} \mathrm{d}z\, \frac{P(z)}{Q(z)} \mathrm{e}^{\pm \mathrm{i}\alpha z} = 0$$

for $i = 1, 2, 3$, where $\tilde{\gamma}_{\pm,i}(R)$ are the curves depicted in Fig. 2. To this end, we parameterize

$$
\begin{aligned}
\tilde{\gamma}_{\pm,1}(R)\colon z &= R \pm \mathrm{i}\sqrt{r}, \quad r \in [0, R] \implies R \leq |z| \leq \sqrt{R^2 + R}, \\
\tilde{\gamma}_{\pm,2}(R)\colon z &= r \pm \mathrm{i}\sqrt{R}, \quad r \in [R, -R] \implies \sqrt{R} \leq |z| \leq \sqrt{R^2 + R}, \\
\tilde{\gamma}_{\pm,3}(R)\colon z &= -R \pm \mathrm{i}\sqrt{r}, \quad r \in [R, 0] \implies R \leq |z| \leq \sqrt{R^2 + R},
\end{aligned}
$$

so that

$$
|\mathrm{e}^{\pm\mathrm{i}\alpha z}| = \begin{cases} \mathrm{e}^{-\alpha\sqrt{r}}, & z \in \tilde{\gamma}_{\pm,1}(R), \\ \mathrm{e}^{-\alpha\sqrt{R}}, & z \in \tilde{\gamma}_{\pm,2}(R), \\ \mathrm{e}^{-\alpha\sqrt{r}}, & z \in \tilde{\gamma}_{\pm,3}(R), \end{cases} \qquad \text{and} \qquad L(\tilde{\gamma}_{\pm,i}(R)) = \begin{cases} \sqrt{R}, & i = 1, \\ 2R, & i = 2, \\ \sqrt{R}, & i = 3. \end{cases}
$$

Hence, Lemma 1 can be used with

$$
M_{\tilde{\gamma}_{\pm,i}(R)} = \sup_{z \in \tilde{\gamma}_{\pm,i}(R)} \left| \frac{P(z)}{Q(z)} \mathrm{e}^{\pm\mathrm{i}\alpha z} \right| \leq \sup_{z \in \tilde{\gamma}_{\pm,i}(R)} \frac{C}{|z|} |\mathrm{e}^{\pm\mathrm{i}\alpha z}| \leq \begin{cases} \sup_{r\in[0,R]} \frac{C}{R} \mathrm{e}^{-\alpha\sqrt{r}}, & i = 1, \\ \sup_{r\in[R,-R]} \frac{C}{\sqrt{R}} \mathrm{e}^{-\alpha\sqrt{R}}, & i = 2, \\ \sup_{r\in[R,0]} \frac{C}{R} \mathrm{e}^{-\alpha\sqrt{r}}, & i = 3, \end{cases}
$$

$$
= \begin{cases} \frac{C}{R}, & i = 1, \\ \frac{C}{\sqrt{R}} \mathrm{e}^{-\alpha\sqrt{R}}, & i = 2, \\ \frac{C}{R}, & i = 3, \end{cases}
$$

leading to

$$
\left| \int_{\tilde{\gamma}_{\pm,i}(R)} \mathrm{d}z\, \frac{P(z)}{Q(z)} \mathrm{e}^{\pm\mathrm{i}\alpha z} \right| \leq M_{\tilde{\gamma}_{\pm,i}(R)} L(\tilde{\gamma}_{\pm,i}(R)) \leq \begin{cases} \frac{C}{\sqrt{R}}, & i = 1, \\ 2C\sqrt{R}\mathrm{e}^{-\alpha\sqrt{R}}, & i = 2, \\ \frac{C}{\sqrt{R}}, & i = 3, \end{cases}
$$

$$
\overset{R\to\infty}{\to} 0.
$$

Since the integrals vanish if their absolute value does, this completes the proof. □

*Two remarks regarding the above proof are in order:* first, had we used a rectangle in the lower (upper) complex half-plane for $f_+(z)$ ($f_-(z)$), the exponential functions would have blown up for $R \to \infty$ and the integrals over $\tilde{\gamma}_{\mp,i}(R)$ would not have vanished, since

$$|\mathrm{e}^{\pm \mathrm{i}\alpha z}| = \begin{cases} \mathrm{e}^{\alpha\sqrt{r}}, & z \in \tilde{\gamma}_{\mp,1}(R), \\ \mathrm{e}^{\alpha\sqrt{R}}, & z \in \tilde{\gamma}_{\mp,2}(R), \\ \mathrm{e}^{\alpha\sqrt{r}}, & z \in \tilde{\gamma}_{\mp,3}(R). \end{cases}$$

Secondly, it is not possible to use an upper (lower) arc in the complex half-plane for $f_+(z)$ ($f_-(z)$) with Lemma 1, as it was done for the proof of Proposition 2, because the resulting estimates are not strong enough, yielding

$$\tilde{M}_{\gamma_\pm(R)} = \sup_{z\in\gamma_\pm(R)} \left|\frac{P(z)}{Q(z)}\mathrm{e}^{\pm\mathrm{i}\alpha z}\right| \le \sup_{z\in\gamma_\pm(R)} \frac{C}{|z|}|\mathrm{e}^{\pm\mathrm{i}\alpha z}| = \sup_{\varphi\in[0,\pi]} \frac{C}{R}\mathrm{e}^{-\alpha R\sin\varphi} = \frac{C}{R}$$

and thus

$$\left|\int_{\gamma_\pm(R)} \mathrm{d}z\, \frac{P(z)}{Q(z)}\mathrm{e}^{\pm\mathrm{i}\alpha z}\right| \le C\pi \ne 0.$$

If, however, $\deg(P) \le \deg(Q) - 2$ holds for the case with the exponential function, it is possible to use the upper/lower arc with Lemma 1 again. Moreover, one can use less restrictive estimates that indeed allow for the use of an upper/lower arc also for the case $\deg(P) \le \deg(Q) - 1$, see JORDAN's lemma [5].

# 2. The HELMHOLTZ Equation's GREEN's Function in Position Space

The object we investigate in these notes is the operator $\hat{G}_0(E) \coloneqq (E - \hat{H}_0 \pm \mathrm{i}\epsilon)^{-1}$ evaluated in position space, with $\hat{H}_0 = \hat{\boldsymbol{p}}^2/(2m)$ being the Hamiltonian of a free particle, *i.e.*,

$$G_\pm(\boldsymbol{x}, \boldsymbol{x}') \coloneqq \frac{\hbar^2}{2m} \langle \boldsymbol{x} \big| (E - \hat{H}_0 \pm \mathrm{i}\epsilon)^{-1} \big| \boldsymbol{x}' \rangle \,.$$

Here, the energy is given by $E = \hbar^2 k^2/(2m)$, with $k = |\boldsymbol{k}|$. The factor of $\hbar^2/(2m)$ has been attached for convenience, as will become clear in the course of the calculation, see also the lecture notes.

We start by making use of the completeness relation in momentum space (twice),

$$\mathbb{1} = \int \frac{\mathrm{d}^3 p}{(2\pi\hbar)^3} \, |\boldsymbol{p}\rangle \langle \boldsymbol{p}| \,,$$

leading to

$$G_\pm(\boldsymbol{x}, \boldsymbol{x}') = \frac{\hbar^2}{2m} \int \frac{\mathrm{d}^3 p}{(2\pi\hbar)^3} \int \frac{\mathrm{d}^3 p'}{(2\pi\hbar)^3} \, \langle \boldsymbol{x}|\boldsymbol{p}\rangle \, \langle \boldsymbol{p}|(E - \hat{H}_0 \pm \mathrm{i}\epsilon)^{-1}|\boldsymbol{p}'\rangle \, \langle \boldsymbol{p}'|\, \boldsymbol{x}'\rangle \,.$$

Since $|\boldsymbol{p}^{(\prime)}\rangle$ is an eigenstate of $\hat{H}_0$ with eigenvalue (energy) $E_0^{(\prime)} = {p^{(\prime)}}^2/(2m)$, where $p^{(\prime)} = |\boldsymbol{p}^{(\prime)}|$, and $\langle \boldsymbol{x}|\boldsymbol{p}\rangle = \mathrm{e}^{\mathrm{i}/\hbar\, \boldsymbol{p}\cdot\boldsymbol{x}} = \langle \boldsymbol{p}|\boldsymbol{x}\rangle^*$, we find

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) = \frac{\hbar^2}{2m}\int \frac{\mathrm{d}^3p}{(2\pi\hbar)^3}\int \frac{\mathrm{d}^3p'}{(2\pi\hbar)^3}\mathrm{e}^{\mathrm{i}/\hbar\, \boldsymbol{p}\cdot\boldsymbol{x}}(E - E_0^{(\prime)} \pm \mathrm{i}\epsilon)^{-1}\, \langle \boldsymbol{p}|\boldsymbol{p'}\rangle\, \mathrm{e}^{-\mathrm{i}/\hbar\, \boldsymbol{p'}\cdot\boldsymbol{x'}}.$$

Using that $\langle \boldsymbol{p}|\boldsymbol{p'}\rangle = (2\pi\hbar)^3\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p'})$ due to the orthogonality of the momentum states and the proper normalization, we obtain

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) = \frac{\hbar^2}{2m}\int \frac{\mathrm{d}^3p}{(2\pi\hbar)^3}\frac{\mathrm{e}^{\mathrm{i}/\hbar\, \boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x'})}}{E - E_0 \pm \mathrm{i}\epsilon}.$$

Performing the change of variables $\boldsymbol{p} = \hbar\boldsymbol{q}$, *i.e.*, $E_0 = \hbar^2q^2/(2m)$, $q = |\boldsymbol{q}|$, we arrive at

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) = \int \frac{\mathrm{d}^3q}{(2\pi)^3}\frac{\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x'})}}{k^2 - q^2 \pm \mathrm{i}\epsilon'},$$

where $\epsilon' = 2m/\hbar^2\,\epsilon$ is still infinitesimally small and takes the role of $\epsilon$. Next, we define the angle $\theta$ by means of $\theta = \angle(\boldsymbol{q},\boldsymbol{x}-\boldsymbol{x'})$, *i.e.*, $\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x'}) = q|\boldsymbol{x}-\boldsymbol{x'}|\cos\theta$, and choose (rotate) the coordinate system such that this angle coincides with the system's polar angle, which can be achieved by having $\boldsymbol{q}$ point into the positive $z$ direction. Transforming to polar coordinates, the above expression then becomes

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) = \frac{1}{(2\pi)^3}\int_0^\infty \mathrm{d}q\, q^2\int_{-1}^1 \mathrm{d}\cos\theta\int_0^{2\pi}\mathrm{d}\phi\,\frac{\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|\cos\theta}}{k^2-q^2\pm\mathrm{i}\epsilon'}.$$

Performing the integrations over the two angles, we finally obtain

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) = \frac{1}{4\pi^2}\frac{1}{\mathrm{i}|\boldsymbol{x}-\boldsymbol{x'}|}\int_0^\infty \mathrm{d}q\, q\frac{\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|} - \mathrm{e}^{-\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{k^2-q^2\pm\mathrm{i}\epsilon'},$$

which, since the integrand is symmetric (even) under $q \to -q$, can be written as an integration over the full real domain with an additional factor of $1/2$,

$$G_\pm(\boldsymbol{x},\boldsymbol{x'}) = -\frac{1}{8\pi^2}\frac{1}{\mathrm{i}|\boldsymbol{x}-\boldsymbol{x'}|}\int_{-\infty}^\infty \mathrm{d}q\, q\frac{\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|} - \mathrm{e}^{-\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q^2-k^2\mp\mathrm{i}\epsilon'}.$$

Note the swap in the sign of the $\pm\mathrm{i}\epsilon'$ term due to the factorized minus sign in the last step.

In order to evaluate this integral, we will make use of the residue theorem. To this end, we define

$$I_\pm(\boldsymbol{x},\boldsymbol{x'}) := \int_{-\infty}^\infty \mathrm{d}q\, q\frac{\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|} - \mathrm{e}^{-\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q^2-k^2\mp\mathrm{i}\epsilon'}$$

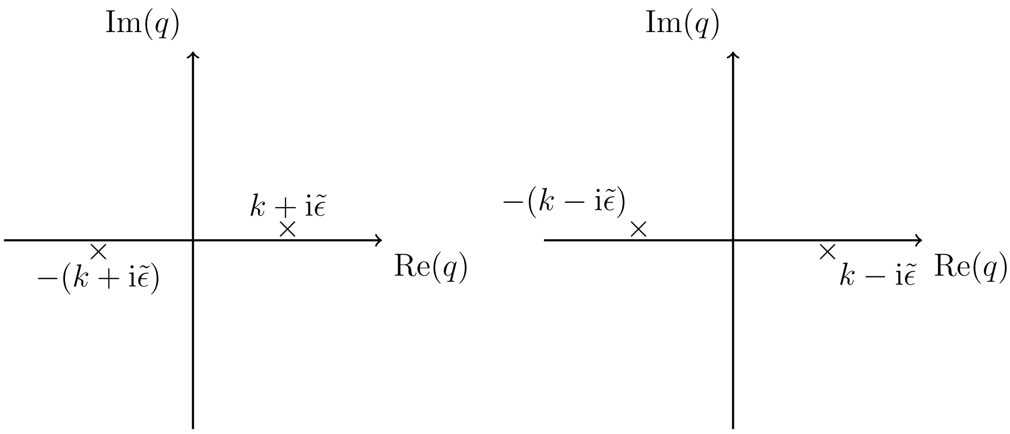


Figure 3: The poles of the integrand defined by $I_+(\boldsymbol{x}, \boldsymbol{x'})$ (*left*) and $I_-(\boldsymbol{x}, \boldsymbol{x'})$ (*right*) in the complex $q$-plane.

and note that the (first-order) poles of the integrand are located at

$$q_{\pm,1} = \sqrt{k^2 \pm \mathrm{i}\epsilon'} = k\sqrt{1 \pm \frac{\mathrm{i}\epsilon'}{k^2}} \approx k\Big(1 \pm \frac{\mathrm{i}\epsilon'}{2k^2}\Big) = k \pm \mathrm{i}\tilde{\epsilon},$$
$$q_{\pm,2} = -\sqrt{k^2 \pm \mathrm{i}\epsilon'} = -k\sqrt{1 \pm \frac{\mathrm{i}\epsilon'}{k^2}} \approx -k\Big(1 \pm \frac{\mathrm{i}\epsilon'}{2k^2}\Big) = -(k \pm \mathrm{i}\tilde{\epsilon}) = -q_{\pm,1},$$

where $\tilde{\epsilon} = \epsilon'/(2k)$ is still infinitesimally small and substitutes the role of $\epsilon'$, see Figure 3. In other words, the denominator can be written as

$$q^2 - k^2 \mp \mathrm{i}\epsilon' = (q - q_{\pm,1})(q + q_{\pm,1}) = [q - (k \pm \mathrm{i}\tilde{\epsilon})][q + (k \pm \mathrm{i}\tilde{\epsilon})].$$

We then make use of Proposition 3 to obtain

$$I_\pm(\boldsymbol{x}, \boldsymbol{x'}) = \lim_{R\to\infty}\Bigg[\oint_{\tilde{\Gamma}_+(R)} \underbrace{\frac{q\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q^2 - k^2 \mp \mathrm{i}\epsilon'}}_{=:F_\pm(q)} - \oint_{\tilde{\Gamma}_-(R)} \underbrace{\frac{q\mathrm{e}^{-\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q^2 - k^2 \mp \mathrm{i}\epsilon'}}_{=:G_\pm(q)}\Bigg],$$

which, using the residue theorem and the fact that only one of the poles lies inside of the integration contour for each integral, see Fig. 3, evaluates to

$$I_\pm(\boldsymbol{x}, \boldsymbol{x'}) = 2\pi\mathrm{i}\Big[\mathrm{Res}[F_\pm(q), \underbrace{\pm(k \pm \mathrm{i}\tilde{\epsilon})}_{=\pm q_{\pm,1}}] + \mathrm{Res}[G_\pm(q), \underbrace{\mp(k \pm \mathrm{i}\tilde{\epsilon})}_{=\mp q_{\pm,1}}]\Big]$$

Here, we used that the winding numbers of $\tilde{\Gamma}_\pm(R)$ around the corresponding poles are given by $\mathrm{ind}_{\tilde{\Gamma}_\pm(R)}(q_{\pm,1/2}) = \pm 1$. Calculating the residues, we thus find

$$
\begin{aligned}
I_\pm(\boldsymbol{x},\boldsymbol{x'}) &= 2\pi\mathrm{i}\underbrace{\left[\left.\frac{q\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q \pm q_{\pm,1}}\right|_{q=\pm q_{\pm,1}} + \left.\frac{q\mathrm{e}^{-\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q \mp q_{\pm,1}}\right|_{q=\mp q_{\pm,1}}\right]}_{=\frac{1}{2}\left[\mathrm{e}^{\pm\mathrm{i}q_{\pm,1}|\boldsymbol{x}-\boldsymbol{x'}|}+\mathrm{e}^{\pm\mathrm{i}q_{\pm,1}|\boldsymbol{x}-\boldsymbol{x'}|}\right]} = 2\pi\mathrm{i}\mathrm{e}^{\pm\mathrm{i}q_{\pm,1}|\boldsymbol{x}-\boldsymbol{x'}|} \\
&\overset{\epsilon\to 0}{\to} 2\pi\mathrm{i}\mathrm{e}^{\pm\mathrm{i}k|\boldsymbol{x}-\boldsymbol{x'}|}.
\end{aligned}
$$

In total, we thus obtain

$$
G_\pm(\boldsymbol{x},\boldsymbol{x'}) = -\frac{1}{8\pi^2}\frac{1}{\mathrm{i}|\boldsymbol{x}-\boldsymbol{x'}|}\underbrace{\int_{-\infty}^{\infty}\mathrm{d}q\, q\frac{\mathrm{e}^{\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}-\mathrm{e}^{-\mathrm{i}q|\boldsymbol{x}-\boldsymbol{x'}|}}{q^2-k^2\mp\mathrm{i}\epsilon'}}_{=I_\pm(\boldsymbol{x},\boldsymbol{x'})} = -\frac{1}{4\pi}\frac{\mathrm{e}^{\pm\mathrm{i}k|\boldsymbol{x}-\boldsymbol{x'}|}}{|\boldsymbol{x}-\boldsymbol{x'}|},
$$

which completes our calculation.

# 3. Summary

In these notes, we calculated the Green's function of the Helmholtz equation in position space,

$$
\begin{aligned}
G_\pm(\boldsymbol{x},\boldsymbol{x'}) &:= \frac{\hbar^2}{2m}\left\langle\boldsymbol{x}\middle|(E-\hat{H}_0\pm\mathrm{i}\epsilon)^{-1}\middle|\boldsymbol{x'}\right\rangle \\
&= -\frac{1}{4\pi}\frac{\mathrm{e}^{\pm\mathrm{i}k|\boldsymbol{x}-\boldsymbol{x'}|}}{|\boldsymbol{x}-\boldsymbol{x'}|},
\end{aligned}
$$

where $E = \hbar^2k^2/(2m)$ and $k = |\boldsymbol{k}|$. In order to do so, we stated and proved three minor theorems from complex analysis, where we abstained from presenting rigorous proofs and focused on comprehensibility instead, aiming at graduate students in physics as readers.

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