CHAPTER 1

BASIC CONCEPTS AND FORMULAS

The main tools in investigation of the Schrödinger equation are methods of functional analysis and theory of distributions: the Fourier transform, the Fredholm Theorem, and the Sobolev Embedding Theorems. In particular, the Fourier transform allows us to obtain an integral representation for the free Schrödinger propagator. The bounds for differential operators and the Sobolev Embedding Theorem extend to the weighted Sobolev spaces using the techniques of pseudodifferential operators.

1 DISTRIBUTIONS AND FOURIER TRANSFORM

A detailed theory of tempered distributions can be found in [24, 40, 41, 72, 78]. It is one of the main tools of the modern theory of partial differential equations.

Definition 1.1. *The Schwartz space of test functions $\mathcal{S} = \mathcal{S}(\mathbb{R}^n)$ is the space of all smooth complex-valued functions $\varphi(x)$ on $\mathbb{R}^n$ with finite seminorms*

$$\|\varphi\|_{N,\alpha} := \sup_{\mathbb{R}^n} \langle x\rangle^N |\partial^\alpha \varphi(x)| < \infty$$

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By Alexander Komech and Elena Kopylova

for all $N > 0$ and all multi-indices $\alpha = (\alpha_1, ..., \alpha_n)$ with $\alpha_k = 0, 1, ...$

Thus, functions in $\mathcal{S}$ with all their derivatives decay faster than the inverse of any polynomial. A sequence φ_k converges to 0 in $\mathcal{S}$ if for all N, α

$$\|\varphi_k\|_{N,\alpha} \to 0, \qquad k \to \infty .$$

Definition 1.2. *The Schwartz space of tempered distributions $\mathcal{S}' = \mathcal{S}'(\mathbb{R}^n)$ is the space of all linear continuous functionals $f : \mathcal{S} \to \mathbb{C}$. By definition,*

$$\langle f, \varphi \rangle := f(\varphi), \quad \varphi \in \mathcal{S} . \tag{1.1}$$

For $f(x) \in C(\mathbb{R}^n)$ or $f(x) \in \mathcal{L}^2 := \mathcal{L}^2(\mathbb{R}^n)$, the corresponding distribution is defined by

$$\langle f, \varphi \rangle := \int f(x)\varphi(x)dx, \quad \varphi \in \mathcal{S} .$$

The Fourier representation for $\psi(x) \in \mathcal{S}(\mathbb{R}^n)$ reads

$$\psi(x) = \frac{1}{(2\pi)^{n/2}} \int e^{i\xi x} \hat{\psi}(\xi) d\xi, \tag{1.2}$$

$$\hat{\psi}(\xi) = F\psi(\xi) := \frac{1}{(2\pi)^{n/2}} \int e^{-i\xi x} \psi(x) dx . \tag{1.3}$$

The Fourier transform F is a linear bicontinuous bijection $\mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$. It can be extended by continuity to tempered distributions by the formula

$$\langle \hat{f}, \phi \rangle := \langle f, \hat{\phi} \rangle , \quad \phi \in \mathcal{S} ,$$

so $F : \mathcal{S}' \to \mathcal{S}'$ is also a linear bicontinuous bijection. Let us note the following basic properties of the Fourier transform in $\mathcal{S}'$:

F1. *For $f \in \mathcal{S}'$*

$$F[\nabla_j f(x)] = i\xi_j Ff(\xi), \quad j = 1, ..., n , \tag{1.4}$$

where $\nabla_j := \dfrac{\partial}{\partial x_j}$.

F2. *$F : \mathcal{L}^2 \to \mathcal{L}^2$ is a unitary operator, and the Plancherel identity holds,*

$$\|\hat{\psi}\| = \|\psi\|, \quad (\psi_1, \psi_2) := \int \psi_1(x)\overline{\psi_2(x)}dx = (\hat{\psi}_1, \hat{\psi}_2) , \tag{1.5}$$

where $\psi, \psi_1, \psi_2 \in \mathcal{L}^2$ and $\|\cdot\|$ stands for the norm in $\mathcal{L}^2$.

F3. *For $\hat{\psi} \in \mathcal{L}^1 := L^1(\mathbb{R}^n)$, formula* (1.2) *remains valid. Similarly, the second formula holds for $\psi \in \mathcal{L}^1$.*

2 FUNCTIONAL SPACES

We will work with various versions of the Sobolev functional spaces. The introduction of the spaces and *weak derivatives* by Sobolev around 1930 resulted later in the Schwartz theory of distributions and turned the theory of partial differential equations into a chapter on modern functional analysis.

2.1 Sobolev spaces

We denote by $\mathcal{H}^s = \mathcal{H}^s(\mathbb{R}^3)$ the Sobolev space for $s \in \mathbb{R}$. For $s = 0, 1, 2, \ldots$ this is the Hilbert space of functions which belong to the $\mathcal{L}^2$ space as well as their distribution derivatives up to the order s. In particular, $\mathcal{H}^0 = \mathcal{L}^2$. For an arbitrary $s \in \mathbb{R}$ the Sobolev space is defined in terms of the Fourier transform: $\mathcal{H}^s$ is the Hilbert space of tempered distributions $\psi(x)$ with the finite norm

$$\|\psi\|_s := \|\langle\xi\rangle^s \hat{\psi}(\xi)\| < \infty\,. \tag{2.1}$$

By the Plancherel identity, the Sobolev norm (2.1) can be written as

$$\|\psi\|_s := \|\langle\nabla\rangle^s \psi\|, \qquad \langle\nabla\rangle^s\psi := F^{-1}\langle\xi\rangle^s\hat{\psi}.$$

Obviously:

i) The embedding $\mathcal{H}^{s_1} \subset \mathcal{H}^{s_2}$ is continuous for $s_1 \geq s_2$.

ii) The scalar product $(\cdot,\cdot)$ in $\mathcal{L}^2$ extends to the duality between $\mathcal{H}^s$ and $\mathcal{H}^{-s}$ for every $s \in \mathbb{R}$:

$$(\psi_1, \psi_2) := (\langle\xi\rangle^s\hat{\psi}_1(\xi), \langle\xi\rangle^{-s}\hat{\psi}_2(\xi)) = \int \hat{\psi}_1(\xi)\overline{\hat{\psi}_2(\xi)}d\xi\,,$$

where $\psi_1 \in \mathcal{H}^s$ and $\psi_2 \in \mathcal{H}^{-s}$.

For any subset $B \subset \mathbb{R}^3$, denote

$$\mathring{\mathcal{H}}^s(B) = \{\psi \in \mathcal{H}^s : \operatorname{supp}\psi \subset \overline{B}\}\,. \tag{2.2}$$

The following Sobolev Embedding Theorems play a crucial role everywhere below.

Theorem 2.1. ([40, Theorem 5.3]) *For any $s > 3/2$ the embedding $\mathcal{H}^s(\mathbb{R}^3) \subset C_b(\mathbb{R}^3)$ is a bounded operator.*

Theorem 2.2. ([40, Theorem 7.2]) *For any bounded subset $B \subset \mathbb{R}^3$ and $s_1 > s_2$, the embedding*

$$\mathring{\mathcal{H}}^{s_1}(B) \subset \mathcal{H}^{s_2}(\mathbb{R}^3) \tag{2.3}$$

is a compact operator.

By definition (see [40, p. 19], [55, p. 233], and [96, p. 277]), embedding (2.3) is compact if

$$\begin{aligned}&\textit{for any } C > 0\textit{, the set } \{\psi \in \mathring{\mathcal{H}}^{s_1}(B) : \|\psi\|_{s_1} \leq C\}\\ &\textit{is contained in a compact subset of } \mathcal{H}^{s_2}(\mathbb{R}^3)\,.\end{aligned} \tag{2.4}$$

2.2 Agmon-Sobolev weighted spaces

For $\sigma \in \mathbb{R}$ denote by $\mathcal{L}^2_\sigma = L^2_\sigma(\mathbb{R}^3)$ the Hilbert space of functions $\psi(x) \in L^2_{\rm loc}(\mathbb{R}^3)$ with the finite norm

$$\|\psi\|_{\mathcal{L}^2_\sigma} := \|\langle x\rangle^\sigma \psi(x)\| < \infty .$$

The weighted norms are a suitable tool for characterization of diverging waves with the conserved L^2-norm. Namely, let us consider a function $\psi(x,t)$ such that

$$\|\psi(x,t)\|_{\mathcal{L}^2_{-\sigma}} \to 0 , \qquad t \to \infty , \tag{2.5}$$

where $\sigma > 3/2$. Then obviously

$$\int_{|x|\le R} |\psi(x,t)|^2 dx \to 0 , \qquad t \to \infty , \tag{2.6}$$

for any $R > 0$. The inverse is true if

$$\int_{\mathbb{R}^3} |\psi(x,t)|^2 dx = \text{const} , \qquad t \in \mathbb{R} . \tag{2.7}$$

Exercise 2.3. *Check that* (2.6) *together with* (2.7) *implies* (2.5).

Further, let us define weighted Agmon-Sobolev spaces. For $s, \sigma \in \mathbb{R}$ we will denote by $\mathcal{H}^s_\sigma = \mathcal{H}^s_\sigma(\mathbb{R}^3)$ the Hilbert space of tempered distributions $\psi(x)$ with the finite norm

$$\|\psi\|_{\mathcal{H}^s_\sigma} := \|\langle\nabla\rangle^s \psi(x)\|_{\mathcal{L}^2_\sigma} < \infty . \tag{2.8}$$

In particular, $\mathcal{H}^0_\sigma = \mathcal{L}^2_\sigma$ and $\mathcal{H}^s_0 = \mathcal{H}^s$. By definition, the operator $(1-\Delta)^p$: $\mathcal{H}^s_\sigma \to \mathcal{H}^{s-2p}_\sigma$ is continuous for any $p, s, \sigma \in \mathbb{R}$. The following lemma will play an important role below.

Lemma 2.4. *For any* $s, \sigma \in \mathbb{R}$:

i) *The operator of multiplication by* $x_j : \mathcal{H}^s_\sigma \to \mathcal{H}^s_{\sigma-1}$ *is continuous.*

ii) *The operator of differentiation* $\partial_j : \mathcal{H}^s_\sigma \to \mathcal{H}^{s-1}_\sigma$ *is continuous.*

Proof. i) We should check that

$$\|x_j\psi\|_{\mathcal{H}^s_{\sigma-1}} \le C\|\psi\|_{\mathcal{H}^s_\sigma} .$$

In other words,

$$\|\langle x\rangle^{\sigma-1}\langle\nabla\rangle^s[x_j\psi(x)]\| \le C\|\langle x\rangle^\sigma\langle\nabla\rangle^s\psi\| . \tag{2.9}$$

Let us denote $f = \langle x\rangle^\sigma\langle\nabla\rangle^s\psi$. Then $\psi = \langle\nabla\rangle^{-s}[\langle x\rangle^{-\sigma} f]$, and hence (2.9) reads

$$\|\langle x\rangle^{\sigma-1}\langle\nabla\rangle^s[x_j\langle\nabla\rangle^{-s}[\langle x\rangle^{-\sigma} f]]\| \le C\|f\| .$$

The product of the operators $\langle x\rangle^{\sigma-1}\langle\nabla\rangle^s x_j\langle\nabla\rangle^{-s}\langle x\rangle^{-\sigma}$ is a continuous operator in $\mathcal{L}^2$ by theorems on composition and boundedness of pseudodifferential operators

(PDOs). The theorems for the classes of PDOs, generated by the operators $\langle x\rangle^\sigma$ and $\langle\nabla\rangle^s$ with any $s,\sigma\in\mathbb{R}$, can be proved by standard PDO technique [3, 40, 77].

ii) The continuity of the operator $\partial_j:\mathcal{H}^s_\sigma\to\mathcal{H}^{s-1}_\sigma$ follows similarly. □

The Sobolev Embedding Theorems 2.1 and 2.2 extend to the weighted Sobolev spaces:

Theorem 2.5. i) *For $s>3/2$ and any $\sigma\in\mathbb{R}$ the embedding $\mathcal{H}^s_\sigma\subset C(\mathbb{R}^3)$ is continuous.*

ii) *For $s_1>s_2$ and $\sigma_1>\sigma_2$ the embedding $\mathcal{H}^{s_1}_{\sigma_1}\subset\mathcal{H}^{s_2}_{\sigma_2}$ is a compact operator.*

2.3 Operator-valued functions

Let H_1 and H_2 be two Hilbert spaces. Denote by $\mathcal{L}(H_1,H_2)$ the space of linear continuous operators $A:H_1\to H_2$ with the norm

$$\|A\|_{H_1\to H_2}:=\sup_{\|\psi\|_{H_1}=1}\|A\psi\|_{H_2}<\infty\,.$$

Let Ω be a subset in $\mathbb{C}$ and $A(\omega):H_1\to H_2$ be an operator-valued function defined for $\omega\in\Omega$.

Definition 2.6. i) *An operator-valued function $A(\omega)$ is* **uniformly continuous** *if*

$$\|A(\omega')-A(\omega)\|_{H_1\to H_2}\to 0\,,\qquad \omega'\to\omega\,,$$

for any $\omega\in\Omega$.

ii) *An operator-valued function $A(\omega)$ is* **strongly continuous** *if $A(\omega)\psi\in C(\Omega,H_2)$ for each $\psi\in H_1$.*

3 FREE PROPAGATOR

The *free Schrödinger equation*

$$i\dot{\psi}(x,t) = -\Delta\psi(x,t)\,, \quad x \in \mathbb{R}^3\,, \tag{3.1}$$

corresponds to the zero potential $V(x) = 0$. Here all the derivatives are understood in the sense of distributions. The solution is defined uniquely by initial condition

$$\psi(x,0) = \psi_0(x)\,, \quad x \in \mathbb{R}^3\,. \tag{3.2}$$

3.1 Fourier transform

A formula for solutions to the *initial problem* (3.1), (3.2) can be calculated by the Fourier transform using the methods of analytic functions. Let us consider solutions $\psi(\cdot,t) \in C(\mathbb{R},\mathcal{L}^2)$ to (3.1), (3.2).

Proposition 3.1. *For every initial data $\psi_0 \in \mathcal{L}^2 \cap \mathcal{L}^1$, the solution $\psi(\cdot,t) \in C(\mathbb{R},\mathcal{L}^2)$ exists and is unique. For $t \in \mathbb{R} \setminus 0$ it is given by*

$$\psi(x,t) = \frac{1}{(4\pi i t)^{3/2}} \int e^{i|x-y|^2/4t}\psi_0(0)dy\,, \qquad \text{a.a. } x \in \mathbb{R}^3\,. \tag{3.3}$$

Proof. *Step* i) After the Fourier transform, (3.1) is equivalent to the ordinary differential equation

$$i\partial_t\hat{\psi}(\xi,t) = \xi^2\hat{\psi}(\xi,t)\,, \quad \xi,t \in \mathbb{R}^3 \times \mathbb{R}\,,$$

in the sense of distributions. Therefore,

$$\partial_t\Big[e^{i\xi^2 t}\hat{\psi}(\xi,t)\Big] = 0\,, \quad \xi,t \in \mathbb{R}^3 \times \mathbb{R}\,, \tag{3.4}$$

and then

$$e^{i\xi^2 t}\hat{\psi}(\xi,t) = C(\xi)\,, \quad \xi,t \in \mathbb{R}^3 \times \mathbb{R}\,, \tag{3.5}$$

where $C(\xi)$ is a tempered distribution of $\xi \in \mathbb{R}^3$. The condition $\psi(\cdot,t) \in C(\mathbb{R},\mathcal{L}^2)$ is equivalent to $\hat{\psi}(\cdot,t) \in C(\mathbb{R},\mathcal{L}^2)$ by property **F2** of the Fourier transform. Hence, setting $t = 0$ in (3.5), we obtain

$$\hat{\psi}_0(\xi) = C(\xi)\,, \quad \xi \in \mathbb{R}^3\,.$$

Finally,

$$\hat{\psi}(\xi,t) = e^{-i\xi^2 t}\hat{\psi}_0(\xi)\,, \quad \xi,t \in \mathbb{R}^3 \times \mathbb{R}\,, \tag{3.6}$$

in the sense of distributions. Obviously, $\hat{\psi}(\cdot,t) \in C(\mathbb{R},\mathcal{L}^2)$ for every $\psi_0 \in \mathcal{L}^2$. Thus the existence and uniqueness of the solution are proved. It remains to prove the integral representation (3.3).

Step ii) First we will prove (3.3) for Im $t < 0$. More precisely, formula (3.6) gives the holomorphic continuation of $\hat{\psi}(\cdot,t)$ from $t \in \mathbb{R}$ to a holomorphic function of $t \in$

$\mathbb{C}^- := \{t \in \mathbb{C} : \text{Im}\ t < 0\}$ with the values in $\mathcal{L}^2$. Respectively, $\psi(\cdot, t) = F^{-1}\hat{\psi}(\cdot, t)$ is also a holomorphic function of $t \in \mathbb{C}^-$ with the values in $\mathcal{L}^2$ by **F2**. Hence, it suffices to calculate the function $\psi(\cdot, t)$ for $t \in \mathbb{C}^-$. In this case $\hat{\psi}(\cdot, t) \in \mathcal{L}^1$. Indeed,

$$|\hat{\psi}(\xi, t)| = |e^{-i\xi^2 t}\hat{\psi}_0(\xi)| \le e^{-\varepsilon\xi^2}|\hat{\psi}_0(\xi)|$$

since $\text{Im}\ t = -\varepsilon < 0$. Hence,

$$\int |\hat{\psi}(\xi, t)| d\xi \le \|e^{-2\varepsilon\xi^2}\| \cdot \|\hat{\psi}_0\| < \infty$$

by the Cauchy-Schwarz inequality. Now property **F3** implies that the inversion of the Fourier transform (3.6) is given by

$$\psi(x, t) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\xi x}\hat{\psi}(\xi, t) d\xi, \quad t \in \mathbb{C}^- . \tag{3.7}$$

Substituting (3.6) into (3.7), we get

$$\psi(x, t) = \frac{1}{(2\pi)^3} \int e^{-i\xi x} e^{-i\xi^2 t}\Big[\int e^{i\xi y}\psi_0(y) dy\Big] d\xi , \tag{3.8}$$

where we have expressed $\hat{\psi}(\xi, 0)$ by (1.3) since $\psi(\cdot, 0) \in \mathcal{L}^1$. By the Fubini Theorem, we can change the order of integration in (3.8) and obtain

$$\psi(x, t) = \int G(t, x, y)\psi_0(y) dy , \qquad G(t, x, y) = \frac{1}{(2\pi)^3} \int e^{-i[\xi(x-y)+\xi^2 t]} d\xi , \tag{3.9}$$

for $t \in \mathbb{C}^-$. The last *Gaussian* integral is calculated in the next section:

$$G(t, x, y) = \frac{1}{(4\pi i t)^{3/2}} e^{-\frac{i(x-y)^2}{4t}} , \quad t \in \mathbb{C}^- . \tag{3.10}$$

Step iii) Finally, let us obtain (3.3) for real $t \neq 0$ taking into account our assumption $\psi_0 \in \mathcal{L}^2 \cap \mathcal{L}^1$. By (3.9) and (3.10), for $x \in \mathbb{R}^3$ and $t \in \mathbb{R} \setminus 0$,

$$\begin{aligned} \psi(x, t - i\varepsilon) \quad &= \quad \frac{1}{(4\pi i(t - i\varepsilon))^{3/2}} \int e^{\frac{i|x-y|^2}{4(t-i\varepsilon)}} \psi_0(y) dy \\ &\to \quad \phi(x, t) := \frac{1}{(4\pi i t)^{3/2}} \int e^{\frac{i|x-y|^2}{4t}} \psi_0(y) dy \end{aligned}$$

since $\psi_0 \in \mathcal{L}^1$. On the other hand, formula (3.6) implies that $\psi(\cdot, t - i\varepsilon) \to \phi(\cdot, t)$ in $\mathcal{L}^2$ for all $t \in \mathbb{R}$. Hence, for some sequence $\varepsilon_k \to 0+$, depending on $t \in \mathbb{R} \setminus 0$,

$$\psi(x, t - i\varepsilon_k) \to \phi(x, t) , \qquad \text{a.a. } x \in \mathbb{R}^3 . \tag{3.11}$$

Therefore,

$$\psi(x, t) = \phi(x, t) , \qquad \text{a.a. } x \in \mathbb{R}^3 , \tag{3.12}$$

which proves (3.3). □

Corollary 3.2. *Formula* (3.3) *implies the estimate*

$$|\psi(x,t)| \leq C|t|^{-3/2}, \quad \text{a.a. } x \in \mathbb{R}^3\,, \tag{3.13}$$

for the solution to the free Schrödinger equation with $\psi_0 \in \mathcal{L}^2 \cap \mathcal{L}^1$.

Exercise 3.3. *Deduce* (3.5) *from* (3.4).
Hint: *For a distribution of* $t \in \mathbb{R}$, *the equation* $f'(t) = 0$ *for* $t \in \mathbb{R}$ *implies that* $f(t) = \text{const}$.

3.2 Gaussian Integrals

It remains to check (3.10). Using elementary algebra, we find that

$$\xi(x-y) + \xi^2 t = t[\xi + \frac{x-y}{2t}]^2 - \frac{(x-y)^2}{4t}\,.$$

Then

$$G(t,x.y) = A(t)e^{-\frac{i(x-y)^2}{4t}}\,, \tag{3.14}$$

where

$$A(t) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{-it[\xi+\frac{x-y}{2t}]^2}d\xi = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{-it\xi^2}d\xi\,.$$

Here we have changed the contour of integration using the Cauchy theorem since the integrals converge for $t \in \mathbb{C}^-$. In the spherical coordinates the last integral reads

$$\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{-it\xi^2}d\xi = \frac{2}{(2\pi)^2}\int_0^\infty e^{-itr^2}r^2dr = \frac{1}{(2\pi)^2}\int_{-\infty}^\infty e^{-itr^2}r^2dr\,.$$

Substituting $z = r(it)^{1/2}$, where we choose $\arg(it)^{1/2} \in (-\pi/4, \pi/4)$ for $t \in \mathbb{C}^-$, we obtain that

$$A(t) = \frac{1}{(2\pi)^2(it)^{3/2}}\int_L e^{-z^2}z^2dz\,, \tag{3.15}$$

where $L = \{z = r(it)^{1/2} : r \in \mathbb{R}\}$ is the contour in the complex plane (see Fig. 1.1). Then

$$\int_L e^{-z^2}z^2dz = \int_{\mathbb{R}} e^{-z^2}z^2dz = \frac{\sqrt{\pi}}{2}\,, \tag{3.16}$$

where the first identity follows from the Cauchy Theorem. Substituting the result into (3.15), and (3.15) into (3.14), we obtain (3.10).

Exercise 3.4. *Check the last identity in* (3.14).
Hint: *Setting* $b_j = \text{Im}\,\dfrac{x_j - y_j}{2t}$ *for* $j = 1,2,3$, *one has for* $t \in \mathbb{C}^-$

$$\begin{aligned}\int_{\mathbb{R}} e^{-it[\xi+\frac{x-y}{2t}]^2}d\xi &= \int_{\mathbb{R}} e^{-it[\xi+ib]^2}d\xi \\ &= \int_{\text{Im }\xi=b} e^{-it\xi^2}d\xi = \int_{\mathbb{R}} e^{-it\xi^2}d\xi\,,\end{aligned} \tag{3.17}$$

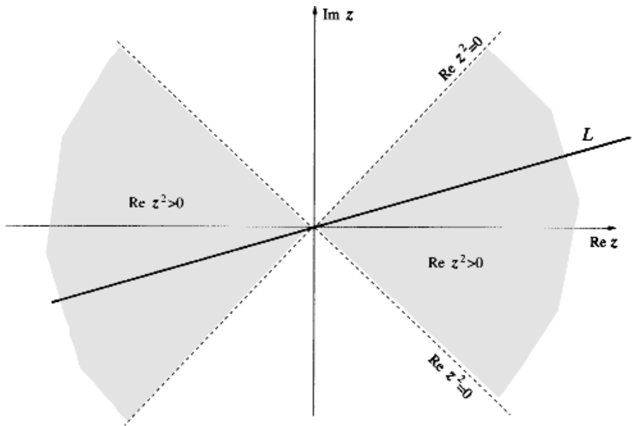

Figure 1.1 The function e^{-z^2} decays in gray sectors.

where the last identity follows from the Cauchy Theorem.

Exercise 3.5. *Check the last identity in* (3.16).
Hint: *Integrate by parts, and obtain*

$$\int_{\mathbb{R}} e^{-z^2} z^2 dz = -\frac{1}{2}\int_{\mathbb{R}} z d e^{-z^2} = \frac{1}{2}\int_{\mathbb{R}} e^{-z^2} dz = \sqrt{\pi}/2\,. \tag{3.18}$$

Exercise 3.6. *Check the last identity in* (3.18).
Hint: *Use the identities*

$$\int_{\mathbb{R}} e^{-x^2} dx \int_{\mathbb{R}} e^{-y^2} dy = \int_{\mathbb{R}^2} e^{-(x^2+y^2)} dx dy = \pi\,, \tag{3.19}$$

where the last identity is obvious in polar coordinates.