Chapter 3

Fourier Transform and Free Hamiltonian

The standard free energy and momentum operators are also properly defined in $\mathbb{R}^n$ through Fourier transform. It is also an opportunity to briefly discuss some aspects of Sobolev spaces and related differential operators. The definitions of distributions $C_0^\infty(\Omega)'$ and tempered distributions $\mathcal{S}'(\Omega)$, as well as their derivatives, are also recalled.

3.1 Fourier Transform

Fourier transform is a very useful tool in dealing with differential operators in $\mathrm{L}^p(\mathbb{R}^n)$, with especial interest in $p = 2$. So some of its main properties will be reviewed and summarized in the first sections, including its relation to Sobolev spaces. Few simple proofs will be presented. Applications to the quantum free particle appear in other sections. Details can be found in the references [Ad75] and [ReeS75]; a nice introduction to distributions and Fourier transform is [Str94]. Readers familiar with the subject are referred to Sections 3.3 and 3.4, which discuss some (quantum) physical quantities.

Recall that the Fourier transform $\mathcal{F} = \hat{\ } : \mathrm{L}^2(\mathbb{R}^n) \to \mathrm{L}^2(\mathbb{R}^n)$ is a unitary operator onto $\mathrm{L}^2(\mathbb{R}^n)$. This is known as the *Plancherel Theorem*, and it implies the *Parseval identity*

$$\|\mathcal{F}\psi\|_2 = \|\psi\|_2, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^n).$$

Note the two notations for the Fourier transform $\mathcal{F}\psi = \hat{\psi}$. For functions $\psi \in \mathrm{L}^1(\mathbb{R}^n)$ there is an explicit expression for this transform, that is,

$$(\mathcal{F}\psi)(p) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\,xp}\,\psi(x)\,dx,$$

with $p = (p_1, \ldots, p_n), x = (x_1, \ldots, x_n) \in \mathbb{R}^n$ and $px = \sum_{j=1}^n p_j x_j$, i.e., the usual inner product in $\mathbb{R}^n$. Denote the norm $|x| = (\sum_{j=1}^n x_j^2)^{1/2}$ and $x^2 = \sum_{j=1}^n x_j^2$. Similarly for the variable p.

Besides the use of variables x and p, sometimes it is convenient to distinguish $\mathrm{L}^2(\mathbb{R}^n)$ from $\mathcal{F}\mathrm{L}^2(\mathbb{R}^n)$ by denoting the latter by $\mathrm{L}^2(\hat{\mathbb{R}}^n)$; functions ψ and operators T acting in $\mathrm{L}^2(\mathbb{R}^n)$ are said to be in the *position representation*, while the corresponding $\hat{\psi}$ and $\hat{T} := \mathcal{F}T\mathcal{F}^{-1}$ acting in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$ are said to be in the *momentum representation*; see Section 3.4 for illustrations that justify the nomenclature.

The inverse Fourier transform $\mathcal{F}^{-1}\mathrm{L}^2(\hat{\mathbb{R}}^n) = \mathrm{L}^2(\mathbb{R}^n)$ has the expression, for $\phi \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$,

$$(\mathcal{F}^{-1}\phi)(x) = \check{\phi}(x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{i\,xp}\, \phi(p)\, dp,$$

again with two different notations. These expressions hold, especially, for functions in the Schwartz space

$$\mathcal{S} = \mathcal{S}(\mathbb{R}^n) = \{\psi \in C^\infty(\mathbb{R}^n) : \lim_{|x|\to\infty} \left| x^m \psi^{(k)}(x) \right| = 0, \forall k, m\},$$

where $m = (m_1, \ldots, m_n)$, $k = (k_1, \ldots, k_n)$ are multiindices,

$$x^m = x_1^{m_1} \cdots x_n^{m_n}, \qquad \psi^{(k)}(x) = \frac{\partial^{k_1} \cdots \partial^{k_n} \psi}{\partial x_1^{k_1} \cdots \partial x_n^{k_n}}(x).$$

Also, $|m| = m_1 + \cdots + m_n$, $|k| = k_1 + \cdots + k_n$ (which should not be confused with the norm $|x|, |p|$ above) and $\partial_j^{k_j}\psi$ may also indicate

$$\partial_j^{k_j}\psi = \frac{\partial^{k_j}\psi}{\partial x_j^{k_j}}.$$

It is possible to show that $\mathcal{F}\mathcal{S} = \mathcal{S}$ (one-to-one). Since $\mathcal{S}$ is a dense subspace of all $\mathrm{L}^p(\mathbb{R}^n)$, $1 \le p < \infty$, any bounded linear operator defined on this space can be uniquely extended to $\mathrm{L}^p(\mathbb{R}^n)$. This holds in particular for the Fourier transform, and it is the usual road for its definition on such spaces. If $p = 2$ one has the Plancherel Theorem, and so many authors consider that this is the natural space of Fourier transforms. Instead of $\mathcal{S}$ it is possible to work with $C_0^\infty(\mathbb{R}^n)$ because this space is also dense in $\mathrm{L}^2(\mathbb{R}^n)$ and also $\mathcal{F}C_0^\infty(\mathbb{R}^n)$ is dense in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$.

Recall the famous integral $\int_{\mathbb{R}} \exp(-t^2)\, dt = \sqrt{\pi}$. A sample of Fourier transform evaluations, which will be used repeated times (e.g., in the proof of Theorem 5.5.1), is

$$\mathcal{F}(e^{-wx - zx^2/2})(p) = \frac{1}{\sqrt{z}}\, e^{w^2/(2z)}\, e^{iwp/z - p^2/(2z)},$$

where $w \in \mathbb{C}$ and the branch of the complex number z with $\mathrm{Re}\, z > 0$ has been chosen so that $\mathrm{Re}\, \sqrt{z} > 0$. It is worth remarking that the linear subspace spanned by all such functions

$$\{e^{-wx-zx^2/2} : w, z \in \mathbb{C}, \mathrm{Re}\, z > 0\}$$

is dense in L^2, and so it is a way to extend (and define) the Fourier transform to every element of L^2. Note that $e^{-x^2/2}$ is an eigenvector of $\mathcal{F}$ with eigenvalue 1 (pick $w = 0$ and $z = 1$). More generally, one has that $(\mathcal{F}^2\psi)(x) = \psi(-x)$, $\forall \psi \in \mathrm{L}^2(\mathbb{R}^n)$, so that every even function is an eigenvector corresponding to this eigenvalue.

For computations it is also useful to invoke the limit in $\mathrm{L}^2(\mathbb{R}^n)$

$$(\mathcal{F}\psi)(p) = \lim_{R\to\infty} \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{|x|\le R} e^{-i\,xp}\, \psi(x)\, dx, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^n),$$

which is usually denoted in the literature by

$$(\mathcal{F}\psi)(p) = \mathrm{l.i.m.}\ \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\,xp}\, \psi(x)\, dx.$$

l.i.m. means "limit in the mean."

Exercise 3.1.1. Let $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and $B_R = \{x \in \mathbb{R}^n : |x| \le R\}$ a closed ball. Show that the function $\psi_R = \psi\chi_{B_R}$ is integrable and so the above explicit expression for the Fourier transform $\hat{\psi}_R$ is valid. This justifies the use of l.i.m. above.

Exercise 3.1.2. Find eigenfunctions of the Fourier transform corresponding to the eigenvalues -1 and $\pm i$.

Many utilities of the Fourier transform come from its property of exchanging multiplication and differentiation, as in the next propositions, whose simple proofs are quite instructive. The roots of those properties are the relations

$$\frac{\partial}{\partial x_j} e^{-i\,xp} = -ip_j\, e^{-i\,xp}, \qquad \frac{\partial}{\partial p_j} e^{-i\,xp} = -ix_j\, e^{-i\,xp}.$$

Proposition 3.1.3. *Let $\psi \in \mathcal{S}$. Then,*

a) $(\mathcal{F}\psi^{(k)})(p) = (-i)^{|k|} p^k \hat{\psi}(p)$.
b) $(\mathcal{F}^{-1}\psi)^{(k)}(x) = i^{|k|} \mathcal{F}^{-1}(p^k \hat{\psi}(p))(x)$.

Proposition 3.1.4. *Let $\psi \in \mathrm{L}^2(\mathbb{R}^n)$. Then, for fixed $y \in \mathbb{R}^n$,*

a) $(\mathcal{F}\psi(x-y))(p) = e^{-iyp}\hat{\psi}(p)$.
b) $\mathcal{F}(e^{ixy}\psi(x))(p) = \hat{\psi}(p-y)$.

Similar properties hold for the inverse Fourier transform.

Proposition 3.1.5. *Let $\psi, \phi \in \mathcal{S}$. Then, for the convolution*

$$(\psi * \phi)(x) := \int_{\mathbb{R}^n} \psi(x-y)\, \phi(y)\, dy = \int_{\mathbb{R}^n} \psi(y)\, \phi(x-y)\, dy$$

one has $\mathcal{F}(\psi * \phi)(p) = (2\pi)^{n/2}\, \hat{\psi}(p)\, \hat{\phi}(p)$.

Exercise 3.1.6. Since $\mathcal{S} \subset \mathrm{L}^1(\mathbb{R}^n)$, by using the above explicit integral representation of the Fourier transform, provide proofs of Propositions 3.1.3, 3.1.4 and 3.1.5.

Exercise 3.1.7. Compute the Fourier transform of the following functions in $\mathrm{L}^1(\mathbb{R})$:

a) $\psi(x) = \chi_{[a,b]}(x)$.
b) For $a > 0$, $\psi(x) = e^{-ax}$ if $x \geq 0$ and $\psi(x) = 0$ if $x < 0$.

Exercise 3.1.8. Parseval identity can be used to compute certain integrals. For $a > 0$, consider the characteristic function $\chi_{[-a,a]}(x)$; compute its Fourier transform $\hat{\chi}_{[-a,a]}$ and use Parseval to show that

$$\int_{\mathbb{R}} \left(\frac{\sin ax}{x}\right)^2 dx = \pi a.$$

It is possible to extend the convolution to spaces $\mathrm{L}^p(\mathbb{R}^n)$ by using Young's inequality, which is now recalled.

Proposition 3.1.9 (Young's Inequality). *Let* $1 \leq p, q, r \leq \infty$ *with* $1/p + 1/q = 1 + 1/r$. *If* $\psi \in \mathrm{L}^p(\mathbb{R}^n)$ *and* $\phi \in \mathrm{L}^q(\mathbb{R}^n)$, *then the convolution* $\psi * \phi \in \mathrm{L}^r(\mathbb{R}^n)$ *and*

$$\|\psi * \phi\|_r \leq \|\psi\|_p \, \|\phi\|_q.$$

The expression for $\psi * \phi$ *is the same as that in Proposition* 3.1.5.

3.2 Sobolev Spaces

In Chapter 2 the particular classes of Sobolev spaces $\mathcal{H}^m(\mathbb{R})$ were recalled via distributional (i.e., weak) derivatives and absolutely continuous functions. A main point is that the existence of sufficiently many weak derivatives in $\mathrm{L}^2(\mathbb{R})$ implies some derivatives in the classical sense. In this section additional properties of suitable Sobolev spaces are collected, and the discussion extended to higher dimensions.

Before going on, for reader's convenience, the definition of distribution and its derivatives are suitably recalled. Let Ω be an open subset of $\mathbb{R}^n$; a sequence $(\phi_j)_j \subset C_0^\infty(\Omega)$ is said to converge to $\phi \in C_0^\infty(\Omega)$ if there is a compact set $K \subset \Omega$ so that the support of ϕ_j is contained in K, $\forall j$, and for each multiindex k the sequence of derivatives $\phi^{(k)} \to \phi^{(k)}$ uniformly. $C_0^\infty(\Omega)$ is called the space of *test functions*.

A distribution u on Ω, is a linear functional on $C_0^\infty(\Omega)$ that are continuous under the above sequential convergence, that is, $u(\phi_j) \to u(\phi)$ whenever $\phi_j \to \phi$ in $C_0^\infty(\Omega)$. Its derivative is the distribution $u^{(k)}$ defined by

$$u^{(k)}(\phi) := (-1)^{|k|} u(\phi^{(k)}), \qquad \forall \phi \in C_0^\infty(\Omega).$$

The space of distributions on Ω is denoted by $C_0^\infty(\Omega)'$.

A distribution u is represented by a function $\psi \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ if

$$u(\phi) = \int_\Omega \psi(x)\,\phi(x)\,dx, \qquad \forall \phi \in C_0^\infty(\Omega),$$

and in this case one usually says that $u = \psi$ in the sense of distributions. Note that $\mathrm{L}^1_{\mathrm{loc}}(\Omega)$ is naturally included in the space of distributions, and this fact suggests the extra terminology *generalized function* for distributions. The fundamental fact here is that if $u \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ and

$$\int_\Omega u(x)\,\phi(x)\,dx = 0, \qquad \forall \phi \in C_0^\infty(\Omega),$$

then $u = 0$ a.e. in Ω. This justifies $u = 0$ in the sense of distributions as well as $u = \psi$ above. The Dirac δ is a well-known example of a distribution that is not represented by any function in $\mathrm{L}^1_{\mathrm{loc}}$.

The statement $u \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ has distributional derivative $u^{(k)} = v \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ means

$$u^{(k)}(\phi) := (-1)^{|k|} \int_\Omega u(x)\,\phi^{(k)}(x)\,dx = \int_\Omega v(x)\,\phi(x)\,dx,$$

for all $\phi \in C_0^\infty(\Omega)$. An important result is discussed in Lemma 2.3.9 and Remark 2.3.10, that is, if Ω is an open connected set and u is a distribution with null derivative, then u is constant.

A sequence of distributions $(u_j)_j$ in $C_0^\infty(\Omega)'$ converges to the distribution u, in the same space, if for every $\phi \in C_0^\infty(\Omega)$ the sequence $(u_j(\phi))_j$ converges in $\mathbb{C}$ to $u(\phi)$.

Example 3.2.1. To illustrate how weak is the notion of convergence of distributions, consider the sequence $u_j(x) = e^{ijx}$ in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$, which has a bad behavior in terms of convergence as a sequence of functions (e.g., it has constant absolute values and it does not converge pointwise to any function). However, for each $\phi \in C_0^\infty(\mathbb{R})$, on integrating by parts

$$\begin{aligned} |u_j(\phi)| &= \left| \int_{\mathbb{R}} e^{ijx}\,\phi(x)\,dx \right| = \left| \frac{1}{j} \int_{\mathbb{R}} e^{ijx}\,\phi'(x)\,dx \right| \\ &\le \frac{C_\phi}{j} \|\phi'\|_\infty \longrightarrow 0 \end{aligned}$$

as $j \to \infty$, where C_ϕ is the Lebesgue measure of the support of ϕ. Hence $u_j \to 0$ in the sense of distributions. The mechanism is the fast oscillations as $j \to \infty$ implying cancellations in the integral.

Example 3.2.2. If $0 \le \psi \in \mathrm{L}^1(\mathbb{R}^n)$ and $\int \psi(x)\,dx = 1$, then $\psi_j(x) := j^n \psi(jx)$ converges to Dirac δ at the origin as $j \to \infty$. Indeed, for $\phi \in C_0^\infty(\mathbb{R}^n)$,

$$\begin{aligned} \psi_j(\phi) &= \int_{\mathbb{R}^n} \psi_j(x)\,(\phi(x) - \phi(0))\,dx + \int_{\mathbb{R}^n} \psi_j(x)\,\phi(0)\,dx \\ &= \int_{\mathbb{R}^n} \psi_j(x)\,(\phi(x) - \phi(0))\,dx + \phi(0), \end{aligned}$$

since $\int \psi_j(x)\,dx = 1$. Now a change of variable gives

$$\int_{\mathbb{R}^n} \psi_j(x)\,(\phi(x)-\phi(0))\,dx = \int_{\mathbb{R}^n} \psi(x)\,(\phi(x/j)-\phi(0))\,dx$$

which vanishes as $j\to\infty$ by dominated convergence. Hence $\psi_j(\phi)\to\phi(0)$ for all $\phi\in C_0^\infty(\mathbb{R}^n)$, that is, $\psi_j\to\delta$ in the sense of distributions.

A sequence $(\psi_j)_j \subset \mathcal{S}(\mathbb{R}^n)$ is said to converge to $\psi\in\mathcal{S}(\mathbb{R}^n)$ if for every polynomial $p:\mathbb{R}^n\to\mathbb{C}$ and all multiindex k, $p\psi_j^{(k)}\to p\psi^{(k)}$ uniformly. A *tempered distribution* u on $\mathbb{R}^n$, is a continuous linear functional on $\mathcal{S}(\mathbb{R}^n)$, that is, $u(\psi_j)\to u(\psi)$ whenever $\psi_j\to\psi$ in $\mathcal{S}(\mathbb{R}^n)$. The space of tempered distributions is denoted by $\mathcal{S}'(\mathbb{R}^n)$. Note that $\mathcal{S}'(\mathbb{R}^n)\subset C_0^\infty(\mathbb{R}^n)'$, so that tempered distributions are indeed distributions.

The exponential function e^x is an example of $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$ function that defines a distribution but not a tempered distribution.

At last the definition of (some) Sobolev spaces! For positive integers m, one defines $\mathcal{H}^m(\Omega)$, for an open $\Omega\subset\mathbb{R}^n$, as the Hilbert spaces of $\psi\in\mathrm{L}^2(\Omega)$ so that the weak derivatives $\psi^{(k)}$ exist and $\psi^{(k)}\in\mathrm{L}^2(\Omega)$ for all $|k|\le m$, and it is considered the norm

$$|||\psi|||_m := \left(\sum_{|k|\le m}\left\|\psi^{(k)}\right\|_2^2\right)^{\frac{1}{2}}.$$

In case $\Omega=\mathbb{R}^n$ the Fourier transform provides another approach to $\mathcal{H}^m(\mathbb{R}^n)$. Proofs of some of the next results will be provided as examples of typical arguments.

Proposition 3.2.3. *Let $\psi\in\mathcal{H}^m(\mathbb{R}^n)$. Then, for $|k|\le m$ one has*

$$\mathcal{F}(\psi^{(k)})(p) = (-i)^{|k|}p^k\hat\psi(p),$$

with $\psi^{(k)}$ denoting distributional derivatives.

Proof. It is enough to consider that only one $k_j\neq 0$; the general case follows by induction. Since the weak derivatives belong to $\mathrm{L}^2(\mathbb{R}^n)$, one can use Plancherel's theorem. Let $\phi\in C_0^\infty(\mathbb{R}^n)$. Then, by Proposition 3.1.3,

$$\begin{aligned}\left\langle \mathcal{F}\psi^{(k_j)}),\hat\phi\right\rangle &= \left\langle \psi^{(k_j)},\phi\right\rangle = (-1)^{k_j}\left\langle \psi,\phi^{(k_j)}\right\rangle \\ &= (-1)^{k_j}\left\langle \hat\psi,\mathcal{F}\phi^{(k_j)}\right\rangle = (-1)^{k_j}\left\langle \hat\psi,(-i)^{k_j}p_j^{k_j}\hat\phi\right\rangle \\ &= \left\langle (-i)^{k_j}p_j^{k_j}\hat\psi,\hat\phi\right\rangle,\end{aligned}$$

and the result follows since $\mathcal{F}C_0^\infty(\mathbb{R}^n)$ is dense in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$. ∎

Corollary 3.2.4. *If $\psi \in \mathcal{H}^m(\mathbb{R}^n)$, then*

$$p^k \hat{\psi}(p) \in \mathrm{L}^2(\hat{\mathbb{R}}^n) \quad \textit{and} \quad \psi^{(k)} = \mathcal{F}^{-1}(-i)^{|k|} p^k \mathcal{F}\psi, \ \forall |k| \le m.$$

Corollary 3.2.4 has a converse statement, but for its proof it is necessary to recall that, for a tempered distributions $u \in \mathcal{S}'(\mathbb{R}^n)$, the Fourier transform $\hat{u}$ is defined by

$$\hat{u}(\phi) = u(\hat{\phi}), \qquad \forall \phi \in \mathcal{S}(\mathbb{R}^n),$$

and due to Proposition 3.1.3 the relation

$$\mathcal{F}(u^{(k)})(p) = (-i)^{|k|} p^k \hat{u}(p)$$

follows. The space $\mathrm{L}^p(\mathbb{R}^n)$ can be identified with a subset of $\mathcal{S}'(\mathbb{R}^n)$ (the inclusion $\mathrm{L}^p(\mathbb{R}^n) \mapsto \mathcal{S}'(\mathbb{R}^n)$ is a continuous injection). With this, a very important characterization will be presented.

Proposition 3.2.5. *The above norm $|||\cdot|||_m$ in $\mathcal{H}^m(\mathbb{R}^n)$ is equivalent to*

$$|||\psi|||'_m := \left(\int_{\mathbb{R}^n} \left(1 + |p|^2\right)^m |\hat{\psi}(p)|^2 \, dp \right)^{\frac{1}{2}}.$$

Proof. Let $\psi \in \mathcal{S}(\mathbb{R}^n)$; since $|p|^k \le (1+|p|^2)^{|k|/2}$, then if $p^k \hat{\psi} \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$ for $|k| \le m$,

$$\begin{aligned} \int_{\mathbb{R}^n} \left|\psi^{(k)}(x)\right|^2 dx = \int_{\mathbb{R}^n} \left|p^k \hat{\psi}(p)\right|^2 dp \le \int_{\mathbb{R}^n} (1+|p|^2)^{|k|} \left|\hat{\psi}(p)\right|^2 dp \\ \le \int_{\mathbb{R}^n} (1+|p|^2)^m \left|\hat{\psi}(p)\right|^2 dp, \end{aligned}$$

and there is a constant $a > 0$ obeying $|||\psi|||_m \le a|||\psi|||'_m$, since $\mathcal{S}(\mathbb{R}^n) \sqsubseteq \mathcal{H}^m(\mathbb{R}^n)$ and the norms are continuous, the latter inequality extends to $\psi \in \mathcal{H}^m(\mathbb{R}^n)$. Conversely, if $\psi \in \mathcal{H}^2(\mathbb{R}^m)$, it follows by the binomial relation that there are positive constants b_j so that

$$(1+|p|^2)^m \left|\hat{\psi}(p)\right|^2 = \sum_{j=0}^{m} b_j |p|^{2j} \left|\hat{\psi}(p)\right|^2$$

and so

$$|||\psi|||'^2_m = \sum_{j=0}^{m} b_j \int_{\mathbb{R}^n} |p|^{2j} \left|\hat{\psi}(p)\right|^2 dp,$$

and because the right-hand side is a linear combination of terms of the form $\|p^k \hat{\psi}(p)\|_2^2$, then, by Proposition 3.2.3, there is $b > 0$ with $|||\psi|||'_m \le b|||\psi|||_m$. The proposition is proved. □

Remark 3.2.6. By using the norm $|||\cdot|||'$, it is possible to define $\mathcal{H}^s(\mathbb{R}^n)$ for any $s \in \mathbb{R}$.

Theorem 3.2.7. *Let u be a tempered distribution in $\mathcal{S}'(\mathbb{R}^n)$. Then the following statements are equivalent:*

1. *u belongs to $\mathcal{H}^m(\mathbb{R}^n)$.*
2. *$u^{(m)} \in \mathrm{L}^2(\mathbb{R}^n)$ (weak derivative).*
3. *$p^k \hat{u}(p) \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$, $\forall |k| \le m$.*
4. *$p^m \hat{u}(p) \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$.*

Moreover, if such statements hold, then $\mathcal{F}(u^{(k)})(p) = (-i)^{|k|} p^k \hat{u}(p)$.

Proof. (*Sketch*) The equivalences $1 \Leftrightarrow 2$ and $3 \Leftrightarrow 4$ will not be discussed here. $1 \Rightarrow 3$ is Corollary 3.2.4. Finally, $3 \Rightarrow 1$ follows by Proposition 3.2.5. □

Some of the above results show that, for $\psi \in \mathrm{L}^2(\mathbb{R}^n)$, the existence of weak derivatives implies integrability properties of $\hat{\psi}$. The next discussion is about differentiability properties.

Lemma 3.2.8. *If $\psi \in \mathrm{L}^1(\mathbb{R}^n)$, then $p \mapsto \hat{\psi}(p)$ is a continuous function and*

$$\|\hat{\psi}\|_\infty = \sup_{p \in \mathbb{R}^n} |\hat{\psi}(p)| \le \frac{1}{(2\pi)^{\frac{n}{2}}} \|\psi\|_1 = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} |\psi(x)|\, dx.$$

Similarly, if $\phi \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$, then $\check{\phi}(x)$ is a continuous function and

$$\|\check{\phi}\|_\infty \le \frac{1}{(2\pi)^{\frac{n}{2}}} \|\phi\|_1.$$

Proof. Write

$$|\hat{\psi}(p+h) - \hat{\psi}(p)| \le \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \left| e^{-i(p+h)x} - e^{-i(p)x} \right| |\psi(x)|\, dx$$

and note that, since ψ is integrable, the right-hand side vanishes by dominated convergence as $h \to 0$; hence $\hat{\psi}(p)$ is continuous. The inequality in the statement of the proposition is immediate. □

Exercise 3.2.9. Verify the inequalities in Lemma 3.2.8.

Proposition 3.2.10. *Let $\psi \in \mathrm{L}^1(\mathbb{R}^n)$. If $x^k \psi(x)$ is integrable for all $|k| \le m$, then $\hat{\psi}^{(k)}$ is a continuous and bounded function, and*

$$(\mathcal{F}\psi)^{(k)} = (-i)^{|k|}\, \mathcal{F}(x^k \psi(x)), \qquad \forall |k| \le m.$$

Proof. It is enough to consider $k_j = 1$ for some j and $k_l = 0$ if $l \ne j$; the general case follows by induction. One has

$$\hat{\psi}(p) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\,xp}\, \psi(x)\, dx.$$

Consider also the differentiation of this integrand with respect to p_j, that is,

$$\phi(p) = \phi(p_j) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} (-ix_j) e^{-i\,xp}\,\psi(x)\,dx;$$

this integral is $\phi(p) = -i\mathcal{F}(x_j\psi)(p)$, which is a continuous function of p_j since, by hypothesis, $x_j\psi(x)$ is integrable (see Lemma 3.2.8). For $p_j \in \mathbb{R}$, denote $\hat{\psi}(p_j)$ the function obtained by keeping fixed p_k for $k \neq j$. By using Fubini's theorem it is found that, for $h \neq 0$,

$$\begin{aligned}\left|\frac{1}{h}[\hat{\psi}(p_j+h) - \hat{\psi}(p_j)] - \phi(p_j)\right| &= \left|\frac{1}{h}\int_0^h [\phi(p_j+r) - \phi(p_j)]\,dr\right| \\ &\le \sup_{|r|\le|h|} |\phi(p_j+r) - \phi(p_j)|\,,\end{aligned}$$

and since $\phi(s)$ is uniformly continuous in any closed interval, the above expression vanishes as $h \to 0$. Therefore, $\partial_{p_j}\hat{\psi}(p) = \phi(p)$. □

Corollary 3.2.11. *If $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ and $p^k\hat{\psi}(p)$ is integrable for all $|k| \le m$, then $\psi^{(k)}$ is a continuous and bounded function, and*

$$\psi^{(k)} = i^{|k|}\,\mathcal{F}^{-1}(p^k\hat{\psi}(p)), \qquad \forall |k| \le m.$$

Proof. This is essentially Proposition 3.2.10 adapted to the inverse Fourier transform. □

The functions $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ are characterized as those that have weak derivatives $\psi^{(k)} \in \mathrm{L}^2(\hat{\mathbb{R}}^n)$ for any $|k| \le m$ and, by a set of results called Sobolev embedding theorems (also called Sobolev lemmas), they become more regular with increasing m. One of such (nontrivial) results is the following one:

Theorem 3.2.12 (Sobolev Embedding). *Let Ω be an open subset of $\mathbb{R}^n$. If $\psi \in \mathcal{H}^m(\Omega)$ and $m > r + \frac{n}{2}$, then $\psi^{(k)}$ is a continuous and bounded function for all $|k| \le r$. Furthermore, in case $\Omega = \mathbb{R}^n$ the inclusion map $\mathcal{H}^m(\mathbb{R}^n) \mapsto C^r(\mathbb{R}^n)$ is bounded.*

By way of illustration, take $n = 1$; it follows that if $\psi \in \mathcal{H}^m(\mathbb{R})$ then $\psi^{(k)}$ are bounded continuous functions for $0 \le k < m$. For $n = 3$ and $\psi \in \mathcal{H}^2(\mathbb{R}^3)$, then $\psi^{(k)}$ is surely continuous only for $k = 0$. In case of bounded open intervals (a, b) one has $C(a, b) \subset \mathcal{H}^1(a, b) \subset C[a, b]$; so, roughly speaking, for $n = 1$ the elements of $\mathcal{H}^1$ are continuous functions that are primitives of functions in L^2.

For the curious readers, Exercise 3.2.13 gives a flavor of how such results can be obtained; of course it does not replace a specific text about Sobolev spaces.

Exercise 3.2.13. The case $m > r + n$ and $\Omega = \mathbb{R}^n$ in Theorem 3.2.12 has a simpler proof. The interested reader may follow the steps ahead to prove this restricted version of the first part of Sobolev's embedding theorem, that is, if $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ and $m > r + n$, then $\psi^{(k)}$ is a continuous and bounded function for all $|k| \le r$.

1. If $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ then, by Corollary 3.2.11, conclude that it is enough to show that $p^k\hat{\psi} \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$, for all $|k| \le r$.
2. Write $p^k\hat{\psi} = \phi_1\phi_2$, with

$$\phi_1(p) = \left(\Pi_{j=1}^k \left(1 + |p_j|^{1+k_j}\right)\right)\hat{\psi}(p), \qquad \phi_2(p) = \frac{p^k}{\Pi_{j=1}^k \left(1 + |p_j|^{1+k_j}\right)},$$

and show that if $|k| \le r$ both ϕ_1 and ϕ_2 belong to $\mathrm{L}^2(\hat{\mathbb{R}}^n)$, so that $\phi_1\phi_2$ is integrable. For ϕ_1, dominate it by a finite sum of integrable functions of the form $|p_j|^{r_j}|\hat{\psi}(p)|$, with $0 \le r_j \le |k|$. For ϕ_2 use Fubini's theorem and note that

$$\frac{|p|^n}{1 + |p|^{1+n}} \le \frac{1}{|p|}$$

for $|p|$ large enough.

Exercise 3.2.14. If $\Omega \subset \mathbb{R}^n$ is a bounded set, show that $\psi(t) = |t|^\alpha$ belongs to $\mathcal{H}^m(\Omega)$ iff $(\alpha - m) > -n/2$.

It is also worth mentioning (see [Ad75]):

Lemma 3.2.15. *Let Ω be an open set in $\mathbb{R}^n$ with a regular bounded boundary. Then the norm $|||\psi|||_m$ in $\mathcal{H}^m(\Omega)$ is equivalent to the norm*

$$[\psi]_m := \left(\|\psi\|_2^2 + \sum_{|k|=m} \left\|\psi^{(k)}\right\|_2^2\right)^{\frac{1}{2}}.$$

Example 3.2.16. As an application of Sobolev's embedding theorem, another proof of Proposition 2.3.20 will be provided. Recall that dom $H = C_0^\infty(a,b) \subset \mathcal{H} = \mathrm{L}^2(a,b)$, $V \in \mathrm{L}^2_{\mathrm{loc}}(a,b)$, $-\infty \le a < b \le \infty$, and

$$(H\psi)(x) = -\psi''(x) + V(x)\psi(x), \qquad \psi \in \mathrm{dom}\ H.$$

The question is to find H^*. If $\psi \in \mathrm{dom}\ H^*$, then $H^*\psi \in \mathrm{L}^2(a,b)$ and for all $\phi \in C_0^\infty(a,b)$,

$$\int_a^b \left(-\phi''(x) + V(x)\phi(x)\right)\psi(x)\,dx = \langle\overline{\phi}, H^*\psi\rangle,$$

that is

$$\int_a^b \phi''(x)\psi(x)\,dx = \int_a^b \phi(x)\ \left(V(x)\psi(x) - H^*\psi\right)\,dx,$$

so that the second distributional derivative of ψ belongs to $\mathrm{L}^2_{\mathrm{loc}}(a,b)$; by Sobolev embedding ψ, ψ' are absolutely continuous functions and

$$\psi'' = V\psi - H^*\psi,$$

that is,

$$\text{dom } H^* = \left\{\psi \in \mathrm{L}^2(a,b) : \psi, \psi' \in \mathrm{AC}(a,b), (-\psi'' + V\psi) \in \mathrm{L}^2(a,b)\right\},$$
$$(H^*\psi)(x) = -\psi''(x) + V(x)\psi(x), \qquad \psi \in \text{dom } H^*.$$

Thereby the proof is complete. □

3.3 Momentum Operator

This section begins with a summary of a very important statement. For $\psi \in \mathcal{H}^m(\mathbb{R}^n)$ there are two equivalent ways of differentiating it: if $|k| \le m$, under Fourier transform the derivative in the sense of distributions $\psi \mapsto \psi^{(k_j)}$ corresponds to the multiplication operator $\hat{\psi} \mapsto (-i)^{k_j} p_j^{k_j} \hat{\psi}$ in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$. It is also worth recalling some integration by parts formulae: if $\psi, \phi \in \mathcal{H}^1(\mathbb{R}^n)$, then

$$\int_{\mathbb{R}^n} \psi(x)\partial_j\phi(x)\,dx = -\int_{\mathbb{R}^n} \partial_j(\psi(x))\,\phi(x)\,dx,$$

and for $\psi, \phi \in \mathcal{H}^2(\mathbb{R}^n)$ then

$$\int_{\mathbb{R}^n} \psi(x)\Delta\phi(x)\,dx = -\int_{\mathbb{R}^n} \nabla\psi(x)\cdot\nabla\psi(x)\,dx.$$

Two particular cases will be discussed in detail: related to the first derivative $P_j\psi = -i\partial_j\psi$, corresponding to the jth component of the quantum momentum operator and, related to the laplacian $H_0\psi = -\Delta\psi = -\sum_{j=1}^n \partial_j^2\psi$, corresponding to the quantum kinetic energy in $\mathrm{L}^2(\mathbb{R}^n)$, discussed in Section 3.4.

In $\mathrm{L}^2(\mathbb{R})$ the quantum momentum operator was previously introduced, in Chapter 2), as dom $P = \mathcal{H}^1(\mathbb{R})$,

$$(P\psi)(x) = -i\psi'(x), \qquad \psi \in \text{dom } P.$$

See Examples 2.3.11 and 2.4.10. By Fourier transform one gets

$$(\mathcal{F}P\psi)(p) = p\hat{\psi}(p) = \mathcal{M}_{\varphi(p)}\hat{\psi}(p), \qquad \varphi(p) = p.$$

Note also that $\mathcal{H}^1(\hat{\mathbb{R}}) = \left\{\hat{\psi} \in \mathrm{L}^2(\hat{\mathbb{R}}) : |||\psi|||_1' < \infty\right\}$, that is,

$$|||\psi|||_1' = \left(\int_{\mathbb{R}} \left(1 + |p|^2\right) |\hat{\psi}(p)|^2\,dp\right)^{\frac{1}{2}} < \infty,$$

which is the graph norm of $\mathcal{M}_{\varphi(p)}$ in $\mathrm{L}^2(\hat{\mathbb{R}})$, and dom $P = \mathcal{F}^{-1}\mathcal{H}^1(\hat{\mathbb{R}})$. Then,

$$(\mathcal{F}P\mathcal{F}^{-1})\hat{\psi}(p) = p\hat{\psi}(p), \qquad (P\psi)(x) = (\mathcal{F}^{-1}p\mathcal{F})\psi(x),$$

and it follows that the momentum operator is unitarily equivalent (via Fourier transform) to this multiplication operator $\mathcal{M}_p$ by a continuous real function. Therefore, see Subsection 2.3.2, it provides another proof that this operator is self-adjoint with no eigenvalues, and that its spectrum is $\mathbb{R}$, since such properties hold for $\mathcal{M}_p$ (see Exercise 2.1.26).

This construction is readily generalized to the jth component of the momentum operator P_j in $\mathrm{L}^2(\mathbb{R}^n)$, given by

$$\mathcal{F}(P_j\psi)(p) = p_j\hat{\psi}(p) = \mathcal{M}_{p_j}\hat{\psi}(p), \qquad 1 \le j \le n,$$

which is also self-adjoint, with no eigenvalues and its spectrum is $\mathbb{R}$. The (total) momentum operator is defined through the gradient

$$P = -i\nabla = -i\,(\partial_1, \dots, \partial_n),$$

i.e., $P = \mathcal{F}^{-1}(p_1, \dots, p_n)\mathcal{F} = (\mathcal{F}^{-1}p_1\mathcal{F}, \dots, \mathcal{F}^{-1}p_n\mathcal{F})$.

3.4 Kinetic Energy and Free Particle

The nonrelativistic quantum *kinetic energy* operator in $\mathrm{L}^2(\mathbb{R}^n)$ (or $\mathrm{L}^2(\Omega)$, Ω an open subset of $\mathbb{R}^n$) is denoted by H_0 and (up to a sign) it is the self-adjoint realization of the laplacian (distributional derivatives), that is, $H_0 = -\Delta$ with domain $\mathcal{H}^2(\mathbb{R}^n)$.

For the one-dimensional case $\mathrm{L}^2(\mathbb{R})$ the kinetic energy corresponds to $\operatorname{dom} H_0 = \mathcal{H}^2(\mathbb{R})$ and $H_0\psi = -\psi''$. By using Fourier transform, this operator is unitarily equivalent to the multiplication operator

$$\mathcal{F}H_0\psi = \mathcal{F}H_0\mathcal{F}^{-1}\mathcal{F}\psi = \mathcal{M}_{p^2}\hat{\psi}.$$

In higher dimensions $\mathrm{L}^2(\mathbb{R}^n)$, $n \ge 2$, an alternative way of defining the kinetic energy operator is $\operatorname{dom} H_0 = \mathcal{H}^2(\mathbb{R}^n)$ and

$$(H_0\psi)(x) = -\Delta\psi(x) = \mathcal{F}^{-1}[p^2\hat{\psi}(p)](x), \qquad \psi \in \operatorname{dom} H_0.$$

That is, it is unitarily equivalent to the multiplication operator $\mathcal{F}H_0\psi = \mathcal{M}_{p^2}\hat{\psi}$ in $\mathrm{L}^2(\hat{\mathbb{R}}^n)$,

$$H_0 = \mathcal{F}^{-1}p^2\mathcal{F}.$$

Since $p \mapsto p^2$ is a positive continuous function, it follows that its spectrum is $\sigma(H_0) = \operatorname{rng} p^2 = [0, \infty)$; see Exercise 2.3.29. Further, H_0 has no eigenvalues.

Note that the unitarity of the Fourier transform allows one to conclude that if $\psi \in \mathrm{L}^2(\mathbb{R}^n)$ with $\Delta\psi \in \mathrm{L}^2(\mathbb{R}^n)$, then $\psi \in \mathcal{H}^2(\mathbb{R}^n)$; see other comments on page 197.

Since only kinetic energy is present (there is no interaction among particles), the operator H_0 is also called the *Schrödinger operator for the free particle.*

Another terminology is *free hamiltonian* or *free Schrödinger operator*. Perturbations of H_0 by a potential energy $V(x)$, resulting in the total energy operator, are considered in other chapters.

Proposition 3.4.1. *The operators T_C, T_S with domains $C_0^\infty(\mathbb{R}^n)$ and $\mathcal{S}(\mathbb{R}^n)$, respectively, both with action $\psi \mapsto -\Delta\psi$, are essentially self-adjoint and*

$$\overline{T_C} = H_0 = \overline{T_S}.$$

In other words, $C_0^\infty(\mathbb{R}^n)$ and $\mathcal{S}(\mathbb{R}^n)$ are cores of H_0.

Proof. If $g \in \mathrm{dom}\; T_C^* \subset \mathrm{L}^2(\mathbb{R}^n)$, then

$$\langle g, -\Delta\psi\rangle = \langle T_C^* g, \psi\rangle, \qquad \forall \psi \in C_0^\infty(\mathbb{R}^n);$$

thus the distributional derivative $-\Delta g = T_C^* g \in \mathrm{L}^2(\mathbb{R}^n)$ and so $g \in \mathcal{H}^2(\mathbb{R}^n)$ and $T_C^* g = -\Delta g = H_0 g$, so that $T_C^* \subset H_0$. Conversely, if $\phi \in \mathcal{H}^2(\mathbb{R}^n)$ then $-\Delta\phi \in \mathrm{L}^2(\mathbb{R}^n)$ and, via integration by parts,

$$\langle \phi, T_C\psi\rangle = \langle \phi, -\Delta\psi\rangle = \langle -\Delta\phi, \psi\rangle, \qquad \forall \psi \in C_0^\infty(\mathbb{R}^n);$$

by definition, $\phi \in \mathrm{dom}\; T_C^*$ and $T_C^*\phi = -\Delta\phi = H_0\phi$, so that $H_0 \subset T_C^*$. Hence $T_C^* = H_0$. Since H_0 is self-adjoint, one has $\overline{T_C} = T_C^{**} = H_0$, and it is found that T_C is essentially self-adjoint.

For T_S, note that $T_C \subset T_S \subset H_0$. Thus, since T_C is essentially self-adjoint, $T_C^* = \overline{T_C} = H_0$, and so $H_0 \subset T_S^* \subset T_C^* = H_0$. Therefore, $T_S^* = H_0$ and T_S is essentially self-adjoint (also $\overline{T_S} = T_S^{**} = H_0$). $\square$

Exercise 3.4.2. Show that $(\mathbf{1} + H_0)\mathcal{S} = \mathcal{S}$.

In view of $H_0 = \mathcal{F}^{-1}p^2\mathcal{F}$, one has

$$R_z(H_0) = \mathcal{F}^{-1}\frac{1}{p^2 - z}\mathcal{F},$$

for the resolvent of H_0 at $z \notin [0,\infty)$ (check this!). The operator of multiplication by the functions

$$\frac{1}{p^2 - z} \qquad \text{and} \qquad e^{-itp^2}$$

correspond to important quantum operators in the momentum representation $\mathrm{L}^2(\hat{\mathbb{R}}^n)$; their actions in the position representation $\mathrm{L}^2(\mathbb{R}^n)$ will be discussed in Subsection 3.4.1 and Section 5.5, respectively.

Exercise 3.4.3. Use Fourier transform to show that for all complex numbers $z \notin [0,\infty)$ the operator $P_j R_z(H_0)$ is bounded for any momentum component P_j.

For a measurable function $f : \mathbb{R} \to \mathbb{C}$ one defines the operator

$$\mathrm{dom}\; f(H_0) = \mathcal{F}^{-1}\mathrm{dom}\; f(p^2), \qquad f(H_0) := \mathcal{F}^{-1}f(p^2)\mathcal{F};$$

since dom $f(p^2)$ is a dense set and $\mathcal{F}$ is unitary, then dom $f(H_0)$ is dense and if $f(p^2)$ is real valued the operator $f(H_0)$ is also self-adjoint – see Subsection 2.3.2. If f is a (essentially) bounded function, then $f(H_0) \in \mathrm{B}(\mathcal{H})$. According to the nomenclature on page 80, $f(p^2)$ is the operator $f(H_0)$ in momentum representation.

In a similar way one defines the function of momentum operators $f(P_j)$ and $f(P)$, the latter with $f : \mathbb{R}^n \to \mathbb{C}$. Note, as before, the abuse of notation by indicating the multiplication operator $\mathcal{M}_{f(p)}$ by just $f(p)$.

Exercise 3.4.4. Verify that if $f(p) = p^k$, $k \in \mathbb{N}$, then the corresponding operator $f(H_0)$ in $\mathrm{L}^2(\mathbb{R})$ is

$$\mathrm{dom}\, f(H_0) = \mathcal{H}^{2k}(\mathbb{R}), \qquad f(H_0)\psi = (-1)^k \psi^{(2k)}.$$

Challenge: What about $\sqrt{H_0}$?

3.4.1 Free Resolvent

In this subsection the resolvent of the free hamiltonian $R_z(H_0)$ in $\mathbb{R}^3$, in position representation, will be computed from its momentum representation $(p^2 - z)^{-1}$. First, a result also of general interest.

Lemma 3.4.5. *If $f \in \mathrm{L}^2(\mathbb{R}^n)$, then the operator $f(P)$ in position representation is an integral operator whose kernel is $1/(2\pi)^{\frac{n}{2}}\, \check{f}(y-x)$, that is, for all $\psi \in \mathrm{L}^2(\mathbb{R}^n)$,*

$$(f(P)\psi)(x) := \mathcal{F}^{-1}\left[f(p)\hat{\psi}(p)\right](x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n} \check{f}(y-x)\psi(y)\, dy.$$

Proof. Since $f\hat{\psi} \in \mathrm{L}^1(\hat{\mathbb{R}}^n)$ there is an explicit expression for its inverse Fourier transform. Fix $x \in \mathbb{R}^n$. Then, since $\mathcal{F}^{-1}$ is unitary and by a simple variation of Proposition 3.1.4,

$$\begin{aligned}(2\pi)^{\frac{n}{2}}\mathcal{F}^{-1}\left[f(p)\hat{\psi}(p)\right](x) &= \int_{\mathbb{R}^n} e^{i\,xp} f(p)\hat{\psi}(p)\, dp \\ &= \left\langle e^{-i\,xp}\overline{f(p)}, \hat{\psi}(p)\right\rangle = \left\langle \mathcal{F}^{-1}(e^{-i\,xp}\overline{f(p)})(y), \psi(y)\right\rangle \\ &= \left\langle \overline{\check{f}(y-x)}, \psi(y)\right\rangle = \int_{\mathbb{R}^n} \check{f}(y-x)\psi(y)\, dy.\end{aligned}$$

This is the desired expression. □

Theorem 3.4.6. *Fix a complex number $z \notin [0,\infty)$. Then the resolvent of the free hamiltonian H_0 in $\mathrm{L}^2(\mathbb{R}^3)$ at z, in position representation, is given by*

$$(R_z(H_0)\psi)(x) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|x-y|}}{|x-y|}\psi(y)\, dy, \qquad \forall \psi \in \mathrm{L}^2(\mathbb{R}^3),$$

with the branch of the square root given by $\mathrm{Im}\,\sqrt{z} > 0$.

Proof. The resolvent is $(R_z(H_0)\psi)(x) = \mathcal{F}^{-1}[f(p)\hat{\psi}(p)](x)$ with $f(p) = (p^2 - z)^{-1}$ which belongs to $\mathrm{L}^2(\mathbb{R}^3)$ (and is also bounded). By Lemma 3.4.5, the resolvent is an integral operator with kernel

$$G_0(x - y; z) := 1/(2\pi)^{\frac{3}{2}}\, \check{f}(x - y).$$

The task now is to compute

$$X = (2\pi)^{3/2}\check{f}(x) = \text{l.i.m.} \int_{\mathbb{R}^3} \frac{e^{i\,xp}}{p^2 - z}\, dp = \lim_{R\to\infty} \int_{|p|\le R} \frac{e^{i\,xp}}{p^2 - z}\, dp.$$

Introduce spherical coordinates $xp = |x||p|\cos\theta$, $r = |p|$, $0 \le \theta \le \pi$, $-\pi \le \vartheta < \pi$ and also $a = \cos\theta$. Then

$$\begin{aligned} X &= \lim_{R\to\infty} \int_0^R \int_{-1}^1 \int_{-\pi}^{\pi} \frac{e^{i\,r|x|a}}{r^2 - z}\, r^2\, d\vartheta da\, dr \\ &= \frac{2\pi}{i\,|x|} \lim_{R\to\infty} \int_{-R}^R \frac{re^{i\,r|x|}}{r^2 - z} dr = \frac{2\pi}{i\,|x|} \lim_{R\to\infty} \int_{C_R} \frac{we^{i\,w|x|}}{(w - \sqrt{z})(w + \sqrt{z})} dw, \end{aligned}$$

where $\operatorname{Im} \sqrt{z} > 0$, C_R is the rectangle in the upper half complex plane, delimited by the vertices $(-R, 0), (R, 0), (R, \sqrt{R}), (-R, \sqrt{R})$, and w the complex integration variable. Then, by residues, one gets

$$X = 2\pi^2\, \frac{e^{i\,\sqrt{z}|x|}}{|x|}, \qquad \operatorname{Im} \sqrt{z} > 0,$$

so that

$$G_0(x - y; z) = \frac{1}{4\pi} \frac{e^{i\,\sqrt{z}\,|x-y|}}{|x - y|}, \qquad \operatorname{Im} \sqrt{z} > 0,$$

and the proof is complete. □

Definition 3.4.7. The function $G_0(x - y; z)$, introduced in the proof of Theorem 3.4.6, is called the three-dimensional *free Green function*. It is the kernel of the free resolvent operator in $\mathrm{L}^2(\mathbb{R}^3)$.

Exercise 3.4.8. Given a potential $V : \mathbb{R}^3 \to \mathbb{R}$, assume that $\psi \in \mathrm{L}^2(\mathbb{R}^3)$ is an eigenfunction of $H_0 + V$ with eigenvalue $\lambda < 0$, that is, $(H_0 + V)\psi = \lambda\psi$ and, also, $V\psi \in \mathrm{L}^2(\mathbb{R}^3)$. Show that

$$\psi(x) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-\sqrt{-\lambda}|x-y|}}{|x - y|}\, V(y)\psi(y)\, dy.$$

This is an integral equation for ψ closely related to the *Lippmann-Schwinger equation* in scattering theory.

Exercise 3.4.9. Check that the kernel of the free resolvent operator in $\mathrm{L}^2(\mathbb{R})$, i.e., the one-dimensional free Green function, at $z \notin [0, \infty)$ is

$$G_0(x - y; z) = \frac{i}{2\sqrt{z}}\, e^{i\sqrt{z}\,|x-y|}, \qquad \text{with } \operatorname{Im} \sqrt{z} > 0.$$

Remark 3.4.10. For dimensions different from one and three, the computation of the free Green function is more difficult to handle; it can be performed in terms of modified Bessel functions of the second kind. The situation is simpler for odd dimensions, since spherical Bessel functions can be employed. Nonetheless, they are not too illuminating. See the full expression in [HiS96] page 164 and details in [CouH53], and for Bessel functions [Wa62].

Exercise 3.4.11. Check that for $\mathrm{L}^2(\mathbb{R}^n)$, $n = 1, 3$, there exists (a.e.) the limit of the free Green function for $z = \lambda + i\varepsilon$, $\lambda > 0$,

$$G_0(x-y; \lambda \pm 0) := \lim_{\varepsilon \to 0^\pm} G_0(x-y; \lambda + i\varepsilon).$$

So the operators $R_{\lambda \pm 0}(H_0)$ are also defined as integral operators with kernels $G_0(x-y; \lambda \pm 0)$. Verify that $R_{\lambda+0}(H_0) \neq R_{\lambda-0}(H_0)$. Are these operators bounded?

Exercise 3.4.12. Write out the one-dimensional harmonic oscillator energy operator (Example 2.3.3) $(H\psi)(x) = -\psi''(x) + x^2\psi(x)$ in the position and momentum representations.

Remark 3.4.13. The kinetic energy, the j-component of the momentum and the total momentum operators in $\mathrm{L}^2(\mathbb{R}^n)$, with all physical constants included, have the expressions

$$H_0 = -\frac{\hbar^2}{2m}\Delta, \qquad P_j = -i\hbar\partial_j, \qquad P = -i\hbar\nabla,$$

respectively. For the Green function in $\mathrm{L}^2(\mathbb{R}^3)$,

$$G_0(x-y; z) = \frac{m}{\hbar^2 2\pi} \frac{1}{|x-y|} \exp\left(i \frac{\sqrt{2mz}}{\hbar} |x-y| \right),$$

while in $\mathrm{L}^2(\mathbb{R})$

$$G_0(x-y; z) = \frac{i}{\hbar} \sqrt{\frac{m}{2z}} \exp\left(i \frac{\sqrt{2mz}}{\hbar} |x-y| \right).$$

Finally, the expression of Fourier transform in $\mathrm{L}^2(\mathbb{R}^n)$ usually employed in quantum mechanics takes the form

$$\hat{\psi}(p) = \frac{1}{(2\pi\hbar)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-i\frac{xp}{\hbar}}\, \psi(x)\, dx.$$

Remark 3.4.14. In the context of quantum mechanics, usually the term "Green function" refers to a representation (e.g., in position or momentum representation) of the resolvent of a self-adjoint operator. The Green function for the hydrogen atom Schrödinger operator was studied in [Ho64] and [Schw64] (see Example 6.2.3).