Chapter 1

Preliminaries

In this chapter we collect concepts and results, which will be essential tools for describing and proving what follows in subsequent chapters. The discussion is brief and few proofs are given; rather we give references to appropriate sources in the literature. Unless mentioned otherwise, our Hilbert spaces are infinite dimensional and over the complex field $\mathbb{C}$.

1.1 Linear operators

We shall assume familiarity with the notions of bounded, closable, closed, symmetric and self-adjoint operators: for a comprehensive treatment of what is needed, see [Edmunds and Evans (1987)]. The following topics and facts are included in any basic coverage, we collect them here for ease of reference as they will be important later.

The first topic concerns von Neumann's theory of extensions of a symmetric operator and the supporting background material. The *numerical range* of a linear operator T with domain $\mathcal{D}(T)$ and range $\mathcal{R}(T)$ in a Hilbert space H is the set

$$\Theta(T) := \{(Tu, u) : u \in \mathcal{D}(T), \|u\| = 1\},$$

where $(\cdot,\cdot)$, $\|\cdot\|$ are, respectively, the inner product and norm of H. It is a convex subset of $\mathbb{C}$ and, hence, so is its closure $\overline{\Theta(T)}$. The complement $\tilde{\Delta}(T) := \mathbb{C} \setminus \overline{\Theta(T)}$, has either one or two connected components. If T is bounded, $\Theta(T)$ is a bounded set and, hence, $\tilde{\Delta}(T)$ is connected; if $\overline{\Theta(T)}$ is an infinite strip, $\tilde{\Delta}(T)$ has two connected components, $\tilde{\Delta}_1(T)$ and $\tilde{\Delta}_2(T)$, say, both being half-planes. Let T be closed, denote by I the identity on H and let $\lambda \in \tilde{\Delta}(T)$. Then $T - \lambda I$ has closed range $\mathcal{R}(T - \lambda I)$ with trivial null space (or kernel) $\mathcal{N}(T - \lambda I)$ and its range has constant co-dimension in each connected component of $\tilde{\Delta}(T)$: in the standard terminology, $T - \lambda I$ is therefore a *semi-Fredholm* operator with zero *nullity*, $\text{nul}(T - \lambda I) := \dim \mathcal{N}(T - \lambda I)$, and constant *deficiency*, $\text{def}(T - \lambda I) := \text{codim}\, \mathcal{R}(T - \lambda I)$, in each of $\tilde{\Delta}_1(T)$ and $\tilde{\Delta}_2(T)$. If T is a closed symmetric operator, $\Theta(T)$ is a closed subinterval of the real line and so $\tilde{\Delta}(T)$ includes the upper and lower half-planes $\mathbb{C}_{\pm}$. In this case the constant values of $\operatorname{def}(T-\lambda I)$ for $\lambda \in \mathbb{C}_\pm$ are called the *deficiency indices* (m_+, m_-) of T :

$$m_\mp(T) := \operatorname{def}(T - \lambda I), \quad \lambda \in \mathbb{C}_\pm$$

and also

$$\operatorname{def}(T - \lambda I) = \dim[\mathcal{R}(T - \lambda I)^\perp] = \operatorname{nul}(T^* - \overline{\lambda} I),$$

where $\perp$ denotes the *orthogonal complement*, and T^* the *adjoint* of T. The closed subspaces $\mathcal{N}_\pm := \mathcal{N}(T^* \mp iI)$ are called the *deficiency subspaces* of T, their dimension being the deficiency indices $m_\pm(T)$. An important result of von Neumann is that if T is a closed symmetric operator, the domain $\mathcal{D}(T^*)$ of its adjoint T^* has the direct sum decomposition

$$\mathcal{D}(T^*) = \mathcal{D}(T) \dotplus \mathcal{N}_+ \dotplus \mathcal{N}_-.$$

This gives

$$\dim\{\mathcal{D}(T^*)/\mathcal{D}(T)\} = m_+(T) + m_-(T), \tag{1.1.1}$$

where $\mathcal{D}(T^*)/\mathcal{D}(T)$ denotes the quotient space.

A closed symmetric operator T is self-adjoint if and only if $\mathcal{R}(T - \lambda I) = \mathcal{R}(T - \overline{\lambda} I) = H$ for some, and consequently all, $\lambda \notin \mathbb{R}$. Therefore T is self-adjoint if and only if $m_+(T) = m_-(T) = 0$. Another consequence of von Neumann's theory of extensions of symmetric operators is that T has a self-adjoint extension if and only if $m_+(T) = m_-(T)$. If T is not closed, but only assumed to be closable, it is said to be *essentially self-adjoint* if its closure $\overline{T}$ is self-adjoint. Equivalently, $\overline{T} = T^*$ is the unique self-adjoint extension of T.

The following Kato–Rellich theorem, concerning the stability of self-adjointness or essential self-adjointness under perturbations will have an important role to play. Recall that a linear operator P in H is said to be *relatively bounded with respect to* T, or T*-bounded*, if $\mathcal{D}(T) \subseteq \mathcal{D}(P)$ and there exist non-negative constants a, b, such that

$$\|Pu\| \le a\|u\| + b\|Tu\|, \quad \text{for all} \quad u \in \mathcal{D}(T). \tag{1.1.2}$$

The infimum of the constants b satisfying (1.1.2) for some $a \ge 0$ is called the T-bound of P. If P is T-bounded, satisfies (1.1.2) and is closable, then $\overline{P}$ is $\overline{T}$-bounded and

$$\|\overline{P}u\| \le a\|u\| + b\|\overline{T}u\|, \quad \text{for all} \quad u \in \mathcal{D}(\overline{T}).$$

P is said to be T*-compact* if $\mathcal{D}(T) \subseteq \mathcal{D}(P)$ and for any sequence $\{u_n\}$ in $\mathcal{D}(T)$ which is such that $\|Tu_n\| + \|u_n\|$ is bounded, $\{Pu_n\}$ contains a convergent subsequence. If we endow $\mathcal{D}(T)$ with its graph norm, namely,

$$\|u\|_T := (\|Tu\|^2 + \|u\|^2)^{1/2},$$

then P is T-compact if its restriction to $\mathcal{D}(T)$ is a compact map from $\mathcal{D}(T)$ into H. If T is self-adjoint, this is equivalent to saying that $P(T+i)^{-1}$ is compact on H.

Theorem 1.1.1. *Let T be a symmetric operator in H and P a symmetric operator, which is T-bounded with T-bound < 1. Then*

(1) if T is self-adjoint, so is $T + P$;
(2) if T is essentially self-adjoint, so is $T + P$ and $\overline{T+P} = \overline{T} + \overline{P}$;
(3) if P is T-compact and T is self-adjoint, then $T + P$ is self-adjoint.

The theorem does not hold in general if P is assumed to have T-bound 1. However, the following is proved by Wüst in [Wüst (1971)]; see also [Kato (1976)], Theorem V.4.6.

Theorem 1.1.2. *Let T be essentially self-adjoint and P a symmetric operator with $\mathcal{D}(T) \subseteq \mathcal{D}(P)$ and $\|Pu\| \leq a\|u\| + \|Tu\|$ for some $a \geq 0$ and all $u \in \mathcal{D}(T)$. Then $T + P$ is essentially self-adjoint.*

1.2 Quadratic forms

In quantum mechanics, the differential operators encountered, like the Schrödinger and Dirac operators, are required by the theory to be self-adjoint in the underlying Hilbert space H. This is often not an easy property to establish, and it is customary to start by first restricting the operator on $C_0^\infty(\mathbb{R}^3)$, for instance, so defining a symmetric operator. If this operator is essentially self-adjoint, then there is no ambiguity about the self-adjoint operator to be taken, since the closure is the unique self-adjoint extension. However, it is often the case that there are many self-adjoint extensions and then physical considerations come into play in selecting the appropriate self-adjoint extension. The physically relevant extension is the Friedrichs extension. This is defined in terms of a symmetric quadratic (or sesquilinear) form associated with the initial symmetric operator; see [Edmunds and Evans (1987)], Chapter IV. More generally, one can start with a symmetric quadratic form t (usually referred to merely as a form), which is densely defined, bounded below and closed in H. Closed means that if $t[u] := t[u, u] \geq \delta\|u\|^2$ for all u in the domain $\mathcal{D}(t)$ of t, then $\mathcal{D}(t)$ endowed with the norm $\|u\|_t := (t - \delta + 1)^{1/2}[u]$ is complete: the form is *closable* if the completion of $\mathcal{D}(t)$ with respect to the aforementioned norm can be identified with a subspace of H, i.e., this completion of $\mathcal{D}(t)$ is continuously embedded in H. We set H_t to be the normed space $(\mathcal{D}(t); \|\cdot\|_t)$: it is in fact an inner-product space as the norm is obviously generated by the inner product $(t - \delta + 1)[\cdot, \cdot]$.

A form p is said to be *relatively bounded with respect to* a form t, or simply *t-bounded*, if $\mathcal{D}(p) \supseteq \mathcal{D}(t)$ and

$$|p[u]| \leq a\|u\|^2 + b|t[u]|, \quad u \in \mathcal{D}(t), \tag{1.2.1}$$

where a, b are non-negative constants. The infimum of the constants b satisfying (1.2.1) for some $a \geq 0$ is called the *t-bound* of p. The analogue of Theorem 1.1.1 for forms is

Theorem 1.2.1. *Let t be a densely defined, symmetric quadratic form, which is bounded below, and p a symmetric form, which is t-bounded with t-bound < 1. Then*

(1) t is closable;
(2) $t+p$ is bounded below;
(3) $t+p$ is closable with the closures of t and $t+p$ having the same domain;
(4) $t+p$ is closed if and only if t is closed.

There is a physically distinguished self-adjoint operator associated with t, given by Kato's first representation theorem:

Theorem 1.2.2. *Let t be a closed, densely defined quadratic form in H, which is bounded below. Then there exists a self-adjoint operator T in H such that*

(1) $u \in \mathcal{D}(T)$ if and only if there exists $f \in H$ such that, for all $v \in \mathcal{D}(t)$,

$$t[u,v] = (f,v)$$

in which case $f = Tu$;
(2) $\mathcal{D}(T)$ is dense in H_t;
(3) if $u \in \mathcal{D}(t), f \in H$ and

$$t[u,v] = (f,v)$$

for all v in a dense subspace of H_t, then $f = Tu$.
The space H_t is referred to as the form domain of T, and is usually denoted by $\mathbb{Q}(T)$.

If T_0 is a given symmetric operator in H which is bounded below, the form

$$t_0[u,v] = (T_0u, v), \quad u, v \in \mathcal{D}(T_0),$$

is closable, densely defined and bounded below and its closure satisfies the first representation theorem. In this case the operator T in the theorem is the *Friedrichs extension* of T_0. It is in fact the restriction of T_0^* to $\mathcal{D}(T_0^*) \cap \mathcal{D}(t)$ and has the same lower bound as T_0.

Suppose now that $t = t_1 + t_2$, with domain $\mathcal{D}(t_1) \cap \mathcal{D}(t_2)$, where t_1, t_2 are densely defined, closed forms, which are bounded below, and that t is also densely defined, closed and bounded below. Then, self-adjoint operators $T,\ T_1,\ T_2$ are associated with the forms $t,\ t_1,\ t_2$. In this case T is called the *form sum* of T_1 and T_2, written $T = T_1 \dot{+} T_2$. If $\mathcal{D}(T_1) \cap \mathcal{D}(T_2)$ is dense in H, the Friedrichs extension of $T_1 + T_2$ is also defined, but in general this differs from the form sum; see [Kato (1976)], Example VI-2.19.

A non-negative self-adjoint operator T has a unique square root $T^{1/2}$ which is also non-negative and self-adjoint. Furthermore, $\mathcal{D}(T)$ is a *core* of $T^{1/2}$, i.e., $\mathcal{D}(T)$ is dense in the Hilbert space $H_+(T^{1/2})$ defined by $\mathcal{D}(T^{1/2})$ with the graph norm

$$\|u\|_{H_+(T^{1/2})} := \left(\|T^{1/2}u\|^2 + \|u\|^2\right)^{1/2} = \|(T+1)^{1/2}u\|.$$

These observations lead to the *second representation theorem*:

Theorem 1.2.3. *Let t be a closed, densely defined, non-negative symmetric form, and let T be the associated self-adjoint operator. Then $\mathcal{D}(t) = \mathcal{D}(T^{1/2})$ and*

$$t[u, v] = (T^{1/2}u, T^{1/2}v), \quad u, v \in \mathcal{D}(T^{1/2}).$$

Thus $\mathbb{Q}(T) = H_+(T^{1/2})$.

The operator $(T + 1)^{1/2}$ is an isometric isomorphism of $H_+(T^{1/2})$ onto H and its adjoint is $(T + 1)^{1/2}$, which is an isometry of H onto $H_-(T^{1/2})$, the completion of H with respect to the norm

$$\|u\|_{H_-(T^{1/2})} = \|((T + 1)^{-1/2}u\|^2.$$

We have the triplet of spaces

$$H_+(T^{1/2}) \hookrightarrow H \hookrightarrow H_-(T^{1/2}), \tag{1.2.2}$$

with embeddings defined by the identification maps, which are continuous and have dense ranges.

Let P be a non-negative, self-adjoint operator, which is a *form-bounded* perturbation of the non-negative self-adjoint operator T in the sense that $\mathbb{Q}(P) \supseteq \mathbb{Q}(T) = H_+(T^{1/2})$, i.e., $\mathcal{D}(P^{1/2}) \supseteq \mathcal{D}(T^{1/2})$ and

$$\|P^{1/2}u\| \le K\|u\|_{H_+(T^{1/2})}$$

for some non-negative constant K. Then P is said to be *form compact, relative to T*, or *form T-compact*, if it is compact from $H_+(T^{1/2})$ to $H_-(T^{1/2})$. Equivalently, this means that $(T + 1)^{-1/2}P(T + 1)^{-1/2} : H \to H$ is compact. Note that, on setting $A = P^{1/2}(T + 1)^{-1/2}$, we have $(T + 1)^{-1/2}P(T + 1)^{-1/2} = A^*A$, which is compact on H if and only if A is compact.

Theorem 1.2.3 yields the *polar decomposition* of a general densely defined, closed operator S acting between two Hilbert spaces H_+ and H_-. In this case

$$s[u, v] := (Su, Sv)_{H_-}, \quad u, v \in \mathcal{D}(S) \subseteq H_+$$

is densely defined, non-negative and closed, since

$$(s + 1)[u] = \|Su\|^2_{H_-} + \|u\|^2_{H_+} = \|u\|^2_{H_+(S)}$$

and $H_+(S)$ is complete. It follows that the non-negative, self-adjoint operator associated with s in Theorem 1.2.3 is $T = S^*S$ and

$$s[u, v] = (T^{1/2}u, T^{1/2}v)_{H_+}, \quad u, v \in \mathcal{D}(T^{1/2}) = \mathcal{D}(S).$$

The operator $T^{1/2} = (S^*S)^{1/2}$ is called the *absolute value* of S and written $|S|$. The *form domain* of a general self-adjoint operator S is defined to be $\mathbb{Q}(|S|)$. The operators $S_\pm := (1/2)(|S| \pm S)$ are called the *positive* and *negative* parts of S. The map

$$|S|u \mapsto Su : \mathcal{R}(|S|) \ \text{ onto } \ \mathcal{R}(S)$$

is an isometry, and extends by continuity to an isometry U from $\overline{\mathcal{R}(|S|)} = \mathcal{N}(|S|)^\perp$ onto $\overline{\mathcal{R}(S)} = \mathcal{N}(S)^\perp$. On setting $Uu = 0$ for $u \in \mathcal{R}(|S|)^\perp = \mathcal{N}(|S|)$, U is a *partial isometry* with *initial set* $\overline{\mathcal{R}(|S|)}$ and *final set* $\overline{\mathcal{R}(S)}$. Its adjoint U^* is a partial isometry with initial set $\overline{\mathcal{R}(S)}$ and final set $\overline{\mathcal{R}(|S|)}$. The formula

$$S = U|S|, \quad \mathcal{D}(S) = \mathcal{D}(|S|), \tag{1.2.3}$$

is called the *polar decomposition* of S. See [Edmunds and Evans (1987)], Section IV.3 for further details.

An elegant way of establishing (1.2.3) and consequent properties, is based on the notion of a *supercharge* in *supersymmetric quantum mechanics*; see [Thaller (1992)] Chapter 5. Abstractly, a supercharge Q is a self-adjoint operator in a Hilbert space $\mathcal{H}$ which anti-commutes with a unitary involution τ defined on $\mathcal{H}$, i.e., τ is a bounded self-adjoint operator on $\mathcal{H}$ which is such that $\tau\tau^* = \tau^*\tau = \tau^2 = I$ and $Q\tau + \tau Q = 0$. The operators $P_\pm = 1/2(1 \pm \tau)$ are orthogonal projections onto subspaces $\mathcal{H}_\pm$ and $\mathcal{H}$ has the orthogonal sum decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. On expressing $u = u_+ + u_-$ as the column vector $(u_+, u_-)^t$, where the superscript denotes the transpose, the standard representation for τ is

$$\tau = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with respect to which, a supercharge Q is an off-diagonal matrix operator. It is readily shown that there is a 1-1 correspondence between densely defined closed operators S acting between $\mathcal{H}_+$ and $\mathcal{H}_-$, and supercharges of the form

$$Q = \begin{pmatrix} 0 & S^* \\ S & 0 \end{pmatrix}$$

on $\mathcal{D}(Q) = \mathcal{D}(S) \oplus \mathcal{D}(S^*)$ in $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. The operator Q is self-adjoint and

$$\mathcal{D}(Q^2) = \{f \in \mathcal{D}(Q) : Qf \in \mathcal{D}(Q)\} = \mathcal{D}(S^*S) \oplus \mathcal{D}(SS^*).$$

Since

$$\mathcal{N}(Q) = \mathcal{N}(S) \oplus \mathcal{N}(S^*),$$

and

$$\mathcal{N}(Q) = \mathcal{N}(Q^2) = \mathbb{R}(Q)^\perp,$$

it follows that

$$\mathcal{N}(S) = \mathcal{N}(S^*S) = \mathcal{R}(S^*)^\perp = \mathcal{R}(S^*S)^\perp \tag{1.2.4}$$

and

$$\mathcal{N}(S^*) = \mathcal{N}(SS^*) = \mathcal{R}(S)^\perp = \mathcal{R}(SS^*)^\perp. \tag{1.2.5}$$

Also, by (1.2.3) and $S^* = |S|U^*$, we have on $\mathcal{N}(Q)^\perp$ that

$$\begin{pmatrix} S^*S & 0 \\ 0 & SS^* \end{pmatrix} = Q^2 = \begin{pmatrix} U^*SS^*U & 0 \\ 0 & US^*SU^* \end{pmatrix}.$$

From this we can infer that S^*S on $(\mathcal{N}(S))^\perp$ is unitarily equivalent to SS^* on $(\mathbb{N}(S^*))^\perp$ and so

$$\sigma(SS^*) \setminus \{0\} = \sigma(SS^*) \setminus \{0\}, \tag{1.2.6}$$

where σ denotes the spectrum. In particular, if $\lambda \neq 0$, is an eigenvalue of S^*S with eigenvector f, then λ is an eigenvalue of SS^* with eigenvector Sf, since

$$SS^*(Sf) = S(S^*Sf) = \lambda Sf.$$

Conversely, if $SS^*g = \lambda g,\ \lambda \neq 0$, then $g \in \mathcal{D}(S^*)$ and $S^*SS^*g = \lambda S^*g$. Hence, $f = S^*g \neq 0$ and satisfies $S^*Sf = \lambda f$. Thus g is of the form $g = Sf$, where f is an eigenvector of S^*S corresponding to λ. See [Thaller (1992)], Section 5.2 for a more comprehensive and detailed discussion.

1.3 Spectra of self-adjoint operators

To fix notation, we recall the basic definitions. The *resolvent set* $\rho(T)$ of a closed operator T in H is the open subset of $\mathbb{C}$ defined by

$$\rho(T) := \{\lambda \in \mathbb{C} : (T - \lambda I)^{-1} \text{ is bounded on } H\};$$

$(T - \lambda I)^{-1}$ is called the *resolvent* of T. The *spectrum* $\sigma(T)$ is the complement $\mathbb{C} \setminus \rho(T)$. If T is self-adjoint, the half-planes $\mathbb{C}_\pm$ lie in $\rho(T)$ and

$$\|(T - \lambda I)^{-1}\| \leq |\text{Im}\lambda|^{-1}, \quad \lambda \notin \mathbb{R}.$$

Hence, the spectrum of a self-adjoint operator is a closed subset of the real line. Its *discrete spectrum* $\sigma_D(T)$ consists of the isolated eigenvalues of finite multiplicity. The complement $\sigma(T) \setminus \sigma_D(T)$ is the *essential spectrum* $\sigma_e(T)$ of T. The essential spectrum is a closed subset of $\mathbb{R}$ and can contain eigenvalues, which are either not isolated or are of infinite multiplicity. The set of all eigenvalues of T is called the *point spectrum* $\sigma_p(T)$. If $\{E(\lambda)\}$ is the (right continuous) spectral family of projections associated with T, then $P(\lambda) := E(\lambda) - E(\lambda - 0) \neq 0$ if and only if λ is an eigenvalue, in which case $P(\lambda)$ is the projection of H onto the eigenspace corresponding to λ. Let H_p denote the closed subspace of H spanned by all the $P(\lambda)H$ and $H_c := H_p^\perp$. It can be shown that $u \in H_c$ if and only if $(E(\lambda)u, u) = \|E(\lambda)u\|^2$ is a continuous function of λ. The spectrum of the restriction of T to H_p is $\sigma_p(T)$ and the spectrum of the restriction of T to H_c is called the continuous spectrum of T and written $\sigma_c(T)$.

It is helpful to subdivide $\sigma_c(T)$ into two parts, determined by the properties of the Borel measure $m_u(S) := (E(S)u, u)$ for $u \in H$, where, for instance, $E([a, b]) = E(b) - E(b - 0)$. The *absolutely continuous (singular)* subspace $H_{ac}(H_s)$ of T is the set of $u \in H$ for which the measure m_u is absolutely continuous (singular). The *absolutely continuous spectrum* $\sigma_{ac}(T)$ (*singular continuous spectrum* $\sigma_{sc}(T)$) of T are the spectra of the restrictions of T to H_{ac}, H_s respectively. It can be shown that H has the orthogonal decomposition $H = H_{ac} \oplus H_{sc} \oplus H_p$ and $H_c = H_{ac} \oplus H_{sc}$. See [Reed and Simon (1978)] for further details.

1.4 Compact operators

A particularly important role for compact self-adjoint operators in spectral analysis is as a tool for locating essential spectra. This is a consequence of a celebrated result of H. Weyl, namely, that if a symmetric operator P is T-compact, where T is self-adjoint, then $\sigma_e(T+P) = \sigma_e(T)$. From this it follows that if T, S are self-adjoint operators and $(T-\lambda I)^{-1} - (S-\lambda I)^{-1}$ is compact for some (and hence all) $\lambda \in \rho(T) \cap \rho(S)$, then $\sigma_e(T) = \sigma_e(S)$. The following two improvements are useful in applications. The first concerns an operator sum and the second a form sum. In the first we use the notion of T^n-compactness, with $T \geq 0$ assumed if $n \notin \mathbb{N}$: an operator P is said to be T^n-*compact* if $\mathcal{D}(P) \supset \mathcal{D}(T)$ and for any sequence $\{u_m\}$ which is such that $\|T^n u_m\|^2 + \|u_m\|^2$ is bounded, then $\{Pu_m\}$ contains a convergent subsequence. In other words, P is compact as a map from $\mathcal{D}(T^n)$ with the graph norm $(\|T^n u\|^2 + \|u\|^2)^{1/2}$ into H or, equivalently, $P(T^n+i)^{-1}$ is compact on H. In the second P is form T^n-*compact*, which means that $T \geq 0$ and $(T+1)^{-n/2}|P|(T+1)^{-n/2}$ is compact in H.

Theorem 1.4.1. *Let T be a self-adjoint operator, P a symmetric operator defined on $\mathcal{D}(T)$, which is T^n-compact for some $n \in \mathbb{N}$, and suppose that $T+P$ is self-adjoint. Then*

$$\sigma_e(T+P) = \sigma_e(T).$$

Gustafson and Weidmann proved in [Gustafson and Weidmann (1969)] that Theorem 1.4.1 for $n \in \mathbb{N}$ is no more general than Schechter's original result in [Schechter (1966)] for the case $n = 2$.

Theorem 1.4.2. *Let T be a positive self-adjoint operator and P a self-adjoint operator with $\mathbb{Q}(P) \equiv \mathbb{Q}(|P|) \supset \mathbb{Q}(T)$. Suppose the form associated with the sum $T+P$ is bounded below and closed on $\mathbb{Q}(T)$ and let S be the form sum $T \dotplus P$. Suppose that at least one of the following is satisfied:*

(1) P is T^n-compact for some $n \in \mathbb{N}$;
(2) $\mathbb{Q}(|P|) \supset \mathbb{Q}(T)$ and $|P|$ is form T^n-compact for some $n \in \mathbb{N}$.

Then $\sigma_e(S) = \sigma_e(T)$.

See [Reed and Simon (1978)] p. 116, Corollary 4.

For semi-bounded, self-adjoint operators, the *max-min principle* quoted in the next theorem is an invaluable analytical and computational tool. In Chapter 4, we shall give a result that establishes a modified version for operators with a spectral gap, and thus, in particular, the Dirac operator. The eigenvalues of the self-adjoint operator T below are counted according to their multiplicity and arranged in increasing order.

Theorem 1.4.3. *Let T be a lower semi-bounded, self-adjoint operator in H and, for each $n \in \mathbb{N}$, define*

$$\mu_n(T) := \sup_{M_{n-1}} \inf_{\substack{\psi \in \mathcal{D}(T) \cap M_{n-1}^{\perp}, \\ \|\psi\| = 1}} (T\psi, \psi), \tag{1.4.1}$$

where the supremum is taken over all linear subspaces M_{n-1} of H of dimension at most $n-1$. Then, for each $n \in \mathbb{N}$, the following hold.

(i) $\mu_n(T) < \lambda_e(T) := \inf\{\lambda \in \sigma_e(T)\}$ if and only if T has at least n eigenvalues less than $\lambda_e(T)$. In this case, $\mu_n(T)$ is the nth eigenvalue of T and the infimum in (1.4.1) is attained when M_{n-1} is the linear span of $e_1, e_2, \cdots, e_n$, where e_j is the eigenvector of T corresponding to the jth eigenvalue.

(ii) $\mu_n(T) = \lambda_e(T)$ if and only if T has at most $n-1$ eigenvalues less than $\lambda_e(T)$, and in this case $\mu_m(T) = \mu_n(T)$ for all $m > n$.

In (1.4.1), (Tu, u) and $\mathcal{D}(T)$ may be replaced by the form and form domain of T, respectively.

For non-negative, self-adjoint operators A, B on a Hilbert space H, we write $A \leq B$ if $\mathbb{Q}(B) \subseteq \mathbb{Q}(A)$ and $a[u] \leq b[u]$ for all $u \in \mathbb{Q}(B)$, where a, b are the forms of A, B, respectively. It follows from the form version of the max-min principle that the eigenvalues $\lambda_n(A), \lambda_n(B), n \in \mathbb{N}$, satisfy $\lambda_n(A) \leq \lambda_n(B)$ for all n and hence $N(\lambda, B) \leq N(\lambda, A)$, where

$$N(\lambda, T) := \sharp\{n : \lambda_n(T) \leq \lambda\};$$

see [Edmunds and Evans (1987)], Lemma X1.2.3.

1.5 Fourier and Mellin transforms

The *Fourier transform* is given by

$$(\mathbb{F}u)(\mathbf{p}) := \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\mathbf{p}\cdot\mathbf{x}} u(\mathbf{x}) d\mathbf{x}, \tag{1.5.1}$$

where $\mathbf{p} \cdot \mathbf{x} = \sum_{j=1}^n p_j x_j$. To analyse and describe some of its important properties we shall use the following standard terminology throughout: for a multi-index $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_n) \in \mathbb{N}_0^n$,

$$D^{\boldsymbol{\alpha}} := \prod_{j=1}^n \left(\frac{1}{i} \frac{\partial}{\partial x_j} \right)^{\alpha_j}, \tag{1.5.2}$$

$$\mathbf{x}^j := \prod_{j=1}^n x_j^{\alpha_j}, \tag{1.5.3}$$

and $|\boldsymbol{\alpha}| = \alpha_1 + \alpha_2 + \cdots + \alpha_n$.

We shall denote by $\mathbf{S}(\mathbb{R}^n)$ the Schwartz space of rapidly decreasing functions, i.e., $u \in \mathbf{S}(\mathbb{R}^n)$ if $u \in C^\infty(\mathbb{R}^n)$ and for every $\ell \in \mathbb{N}_0$ and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_n) \in \mathbb{N}_0^n$, there exists a positive constant $K(\boldsymbol{\alpha}, \ell)$ such that

$$|\mathbf{x}|^\ell |D^{\boldsymbol{\alpha}} u(\mathbf{x})| \le K(\boldsymbol{\alpha}, \ell).$$

The Fourier transform has the following well-known properties (see [Weidmann (1980)], Chapter 10):

(i) $\mathbb{F}$ is a linear bijection of $\mathbf{S}(\mathbb{R}^n)$ onto itself and its inverse is given by

$$\left(\mathbb{F}^{-1} v\right)(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i\mathbf{x}\cdot\mathbf{p}} v(\mathbf{p}) d\mathbf{p}. \tag{1.5.4}$$

Moreover, $(\mathbb{F}^{-1} v)(\mathbf{x}) = (\mathbb{F} v)(-\mathbf{x})$ and $\mathbb{F}^4 = I$, the identity on $\mathbf{S}(\mathbb{R}^n)$.

(ii) For $v \in \mathbf{S}(\mathbb{R}^n)$ and $\boldsymbol{\alpha} \in \mathbb{N}^n$

$$\{\mathbb{F} D^{\boldsymbol{\alpha}} \mathbb{F}^{-1}\} v(\mathbf{p}) = \mathbf{p}^{\boldsymbol{\alpha}} v(\mathbf{p}). \tag{1.5.5}$$

(iii) $\mathbb{F}$ has a unique extension, which is a unitary operator on $L^2(\mathbb{R}^n)$. We shall continue to call this unitary operator the Fourier transform and to write it as $\mathbb{F}$. We therefore have

$$\mathbb{F}^{-1} = \mathbb{F}^*. \tag{1.5.6}$$

In particular, this gives the *Parseval formula*

$$(u, v)_{L^2(\mathbb{R}^n)} = (\mathbb{F}u, \mathbb{F}v)_{L^2(\mathbb{R}^n)}. \tag{1.5.7}$$

(iv) $\mathbb{F}$ and $\mathbb{F}^{-1}$ are continuous injections of $L^1(\mathbb{R}^n)$ into the space of bounded continuous functions on $\mathbb{R}^n$ with the supremum norm:

$$\sup_{\mathbf{p}\in\mathbb{R}^n} |(\mathbb{F}f)(\mathbf{p})| \le \frac{1}{(2\pi)^{n/2}} \|f\|_{L^1(\mathbb{R}^n)}, \quad \sup_{\mathbf{x}\in\mathbb{R}^n} |(\mathbb{F}^{-1}f)(\mathbf{x})| \le \frac{1}{(2\pi)^{n/2}} \|f\|_{L^1(\mathbb{R}^n)}.$$

(v) For $f, g \in \mathbf{S}(\mathbb{R}^n)$, define the *convolution* $f * g$ by

$$\begin{aligned}(f * g)(\mathbf{x}) &:= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} f(\mathbf{y}) g(\mathbf{x} - \mathbf{y}) d\mathbf{y} \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} f(\mathbf{x} - \mathbf{y}) g(\mathbf{y}) d\mathbf{y} = (g * f)(x).\end{aligned} \tag{1.5.8}$$

Then

$$\mathbb{F}(f * g) = \widehat{f}\widehat{g}, \tag{1.5.9}$$

where $\widehat{f} = \mathbb{F}f$. If $f, g \in L^1(\mathbb{R}^n), f * g$ is well-defined and belongs to $L^1(\mathbb{R}^n)$, and (1.5.9) continues to hold. Also, if $f, g \in L^2(\mathbb{R}^n), \widehat{f}\widehat{g} \in L^2(\mathbb{R}^n)$ if and only if $f * g \in L^2(\mathbb{R}^n)$ and in this case

$$f * g = \mathbb{F}^{-1}(\widehat{f}\widehat{g}). \tag{1.5.10}$$

We also have

$$\mathbb{F}(fg) = \widehat{f} * \widehat{g}. \tag{1.5.11}$$

The Fourier transform can also be defined on distributions; see [Stein and Weiss (1971)]. It is sufficient for our needs to consider linear functionals on $\mathbf{S}(\mathbb{R}^n)$ of the form

$$u(\phi) = \int_{\mathbb{R}^n} u(\mathbf{x})\phi(\mathbf{x})d\mathbf{x}, \quad \phi \in \mathbf{S}(\mathbb{R}^n),$$

where $u(\cdot)/(1 + |\cdot|^2)^k \in L^1(\mathbb{R}^n)$ for some positive integer k. Such a u lies in the space $\mathbf{S}'(\mathbb{R}^n)$ of *tempered* distribution. The Fourier transform $\hat{u}$ is an element of $\mathbf{S}'(\mathbb{R}^n)$ defined by

$$\hat{u}(\phi) = u(\hat{\phi}), \quad \phi \in \mathbf{S}(\mathbb{R}^n).$$

The convolution $u * \phi$ for $u \in \mathbf{S}'(\mathbb{R}^n), \phi \in \mathbf{S}(\mathbb{R}^n)$ is defined by

$$(u * \phi)\psi = u(\tilde{\phi} * \psi), \quad \psi \in \mathbf{S}(\mathbb{R}^n),$$

where $\tilde{\phi}(\mathbf{x}) = \phi(-\mathbf{x})$ and an analogue of (1.5.10) holds, namely,

$$\mathbb{F}(u * \phi) = \hat{u}\hat{\phi}, \quad u \in \mathbf{S}'(\mathbb{R}^n), \quad \phi \in \mathbf{S}(\mathbb{R}^n) \tag{1.5.12}$$

in the sense that

$$[\mathbb{F}(u * \phi)]\psi = (\hat{u}\hat{\phi})\psi, \quad \psi \in \mathbf{S}(\mathbb{R}^n).$$

The following important examples will be needed later.

Example 1 Let $f(\mathbf{x}) = e^{-\frac{1}{2}|\mathbf{x}|^2}$. Then $\hat{f} = f$ and for $a > 0$,

$$[\mathbb{F}(e^{-\pi a|\cdot|^2})](\mathbf{p}) = \frac{1}{(2\pi a)^{n/2}} e^{-|\mathbf{p}|^2/4\pi a}. \tag{1.5.13}$$

Proof. By Fubini's Theorem, for all $\mathbf{p} \in \mathbb{R}^n$,

$$\begin{aligned}
\hat{f}(\mathbf{p}) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \exp\{-i\mathbf{p}\cdot\mathbf{x} - (1/2)|\mathbf{x}|^2\}d\mathbf{x} \\
&= \prod_{j=1}^n \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}} \exp\{-ip_jx_j - (1/2)x_j^2\}dx_j \\
&= \prod_{j=1}^n \frac{1}{(2\pi)^{n/2}} e^{-\frac{1}{2}p_j^2} \int_{\mathbb{R}} \exp\{-\frac{1}{2}(x_j + ip_j)^2\}dx_j.
\end{aligned}$$

It follows that $\hat{f} = f$ since, by Cauchy's Theorem from complex analysis,

$$\int_{\mathbb{R}} \exp\{-\frac{1}{2}(x_j + ip_j)^2\}dx_j = \int_{\mathbb{R}} \exp\{-\frac{1}{2}x_j^2\}dx_j = \sqrt{2\pi}.$$

The identity (1.5.13) follows by a change of variables. □

Example 2 For $0 < \alpha < n$ and $c_\alpha = (2)^{\alpha/2}\Gamma(\alpha/2)$ where Γ is the Gamma function,

$$\mathbb{F}(|\cdot|^{\alpha-n}) = \frac{c_\alpha}{c_{n-\alpha}}|\cdot|^{-\alpha}, \tag{1.5.14}$$

in the sense that for all $\phi \in \mathbf{S}(\mathbb{R}^n)$,

$$\frac{c_\alpha}{c_{n-\alpha}}\mathbb{F}^{-1}[|\cdot|^{-\alpha}\hat{\phi}](\mathbf{x}) = \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n}|\mathbf{x}-\mathbf{y}|^{\alpha-n}\phi(\mathbf{y})d\mathbf{y}. \tag{1.5.15}$$

In particular, with $n = 3$ and $\alpha = 2$,

$$\mathbb{F}(|\cdot|^{-1})(\mathbf{p}) = \sqrt{2/\pi}|\mathbf{p}|^{-2}, \tag{1.5.16}$$

in the sense that, for all $\phi \in \mathbf{S}$,

$$\mathbb{F}^{-1}[|\cdot|^{-2}\hat{\phi}](\mathbf{x}) = \frac{1}{4\pi}\int_{\mathbb{R}^n}|\mathbf{x}-\mathbf{y}|^{-1}\phi(\mathbf{y})d\mathbf{y}. \tag{1.5.17}$$

Proof. Let $\phi \in \mathbf{S}(\mathbb{R}^n)$. We shall give the proof from [Lieb and Loss (1997)], Theorem 5.9, based on the identity

$$\begin{aligned}\int_0^\infty e^{-\pi kt}t^{\alpha/2-1}dt &= (\pi k)^{-\alpha/2}\int_0^\infty e^{-t}t^{\alpha/2-1}dt \\ &= (2\pi)^{-\alpha/2}c_\alpha k^{-\alpha/2}\end{aligned}$$

which follows by change of variable. Also, on using (1.5.10) and (1.5.13), we have

$$\begin{aligned}\int_{\mathbb{R}^n} e^{i\mathbf{x}\cdot\mathbf{p}}[e^{-\pi|\mathbf{p}|^2t}\hat{\phi}(\mathbf{p})]d\mathbf{p} &= (2\pi)^{n/2}\mathbb{F}^{-1}[e^{-\pi|\cdot|^2t}\hat{\phi}](\mathbf{x}) \\ &= (2\pi)^{n/2}\left(\mathbb{F}^{-1}[e^{-\pi|\cdot|^2t}]*\phi\right)(\mathbf{x}) \\ &= t^{-n/2}\left[e^{-|\cdot|^2/4\pi t}*\phi\right](\mathbf{x}).\end{aligned}$$

From these last two identities and Fubini's Theorem we derive

$$\begin{aligned}(2\pi)^{(n-\alpha)/2}c_\alpha\mathbb{F}^{-1}[|\cdot|^{-\alpha}\hat{\phi}](\mathbf{x}) &= \int_{\mathbb{R}^n} e^{i\mathbf{x}\cdot\mathbf{p}}\left(\int_0^\infty e^{-\pi|\mathbf{p}|^2t}t^{\alpha/2-1}dt\right)\hat{\phi}(\mathbf{p})d\mathbf{p} \\ &= \frac{1}{(2\pi)^{n/2}}\int_0^\infty t^{(\alpha-n)/2-1}\left[\int_{\mathbb{R}^n} e^{-|\mathbf{x}-\mathbf{y}|^2/4\pi t}\phi(\mathbf{y})d\mathbf{y}\right]dt \\ &= \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n}\left(\int_0^\infty t^{(\alpha-n)/2-1}e^{-|\mathbf{x}-\mathbf{y}|^2/4\pi t}dt\right)\phi(\mathbf{y})d\mathbf{y} \\ &= \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n}\left(\int_0^\infty t^{(n-\alpha)/2-1}e^{-|\mathbf{x}-\mathbf{y}|^2t/4\pi}dt\right)\phi(\mathbf{y})d\mathbf{y} \\ &= (2\pi)^{-\alpha/2}c_{n-\alpha}\int_{\mathbb{R}^n}|\mathbf{x}-\mathbf{y}|^{\alpha-n}\phi(\mathbf{y})d\mathbf{y}.\end{aligned}$$

Note that (1.5.15) is consistent with (1.5.12). For on setting $u(\mathbf{x}) = |\mathbf{x}|^{\alpha-n},\ \hat{u}(\mathbf{x}) = (c_\alpha/c_{n-\alpha})|\mathbf{x}|^{-\alpha}$, we have that $u, \hat{u} \in \mathbf{S}'(\mathbb{R}^n)$ and for all $\phi, \psi \in \mathbf{S}(\mathbb{R}^n)$,

$$\begin{aligned}[\mathbb{F}(u*\phi)]\psi &= u(\tilde{\phi}*\hat{\psi}) \\ &= \int_{\mathbb{R}^n} v(\mathbf{x})\hat{\psi}(\mathbf{x})d\mathbf{x} \\ &= \hat{v}(\psi)\end{aligned}$$

where

$$v(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} u(\mathbf{y})\phi(\mathbf{x}-\mathbf{y})d\mathbf{y} = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} |\mathbf{x}-\mathbf{y}|^{\alpha-n}\phi(\mathbf{y})d\mathbf{y}.$$

Hence (1.5.15) implies that $\hat{u}\hat{\phi} = \hat{v}$. □

The *Mellin transform* $\mathcal{M}$ is defined on $L^2(\mathbb{R}_+)$ with Lebesgue measure dx by

$$\psi^\sharp(s) := \mathcal{M}\psi(s) = \frac{1}{\sqrt{2\pi}} \int_0^\infty t^{-1/2-is}\psi(t)dt, \quad s \in \mathbb{R}. \tag{1.5.18}$$

It is a unitary map from $L^2(\mathbb{R}_+)$ onto $L^2(\mathbb{R})$ and has inverse

$$\mathcal{M}^{-1}\psi^\sharp(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty s^{-1/2+it}\psi^\sharp(s)ds, \quad t \in \mathbb{R}_+. \tag{1.5.19}$$

Moreover, with respect to the *convolution*

$$(\psi \star \phi)(s) := \frac{1}{\sqrt{2\pi}} \int_0^\infty \psi(t)\phi(s/t)dt/t,$$

on $L^2(\mathbb{R}_+)$, the Mellin transform satisfies

$$[\mathcal{M}(\psi \star \phi)](s) = \psi^\sharp(s)\phi^\sharp(s). \tag{1.5.20}$$

We shall need the Mellin transform of the function $\tilde{Q}_l(x) := Q_l\left(\frac{1}{2}[x+\frac{1}{x}]\right),\ l \in \mathbb{N}_0$, where Q_l is the Legendre function of the second kind, namely

$$Q_l(z) := \frac{1}{2}\int_{-1}^1 \frac{P_l(t)}{z-t}dt,$$

and P_l is the Legendre polynomial. The following formula is established in [Yaouanc *et al.* (1997)], Section VI; see also [Magnus *et al.* (1966)], p. 72, 8.17.

$$[\mathcal{M}(\tilde{Q}_l)](s) = \sqrt{\frac{\pi}{2}}V_l(s+i/2), \tag{1.5.21}$$

where

$$V_l(z) = \frac{1}{2}\frac{\Gamma([l+1-iz]/2)\Gamma([l+1+iz]/2)}{\Gamma([l+2-iz]/2)\Gamma([l+2+iz]/2)}. \tag{1.5.22}$$

It has the expansion

$$V_l(z) = \frac{2}{\pi}\sum_{j=0}^\infty \frac{\Gamma(n+1/2)\Gamma(n+l+1)}{\Gamma(n+1)\Gamma(n+l+3/2)}\frac{2n+l+1}{(2n+l+1)^2+z^2}, \tag{1.5.23}$$

see [Oberhettinger (1974)], p. 5.

It is instructive to verify (1.5.21) and (1.5.22) by the method in [Yaouanc *et al.* (1997)]. By the definition, (1.5.21) is satisfied with

$$V_l(z) = \frac{1}{\pi}\int_0^\infty x^{-1-iz}\tilde{Q}_l(x)dx.$$

From Rodrigues' formula

$$P_l(t) = \frac{1}{2^l l!}(-1)^l \frac{d^l}{dx^l}(1-x^2)^l,$$

it follows by integration by parts that

$$\tilde{Q}_l(x) = \int_{-1}^{1} \frac{(1-t^2)^l}{[(x+x^{-1})-2t]^{l+1}} dt.$$

The substitution $y = [(x+x^{-1})-2t]/(1-t^2)$ yields

$$\begin{aligned} \tilde{Q}_l(x) &= \int_{\max(x,1/x)} y^{-l-1}(y-x)^{-1/2}(y-1/x)^{-1/2} dy \\ &= \int_0^\infty y^{-1} F(yx) F(y/x) dy, \end{aligned} \tag{1.5.24}$$

where $F(t) = \theta(t-1)t^{-l/2}(t-1)^{-1/2}$ and θ is the Heaviside function: $\theta(t) = 1$ for $t > 0$ and is otherwise 0. Thus, with $G(x) := F(1/x)$,

$$\begin{aligned} V_l(z) &= \frac{1}{2\pi}\int_0^\infty t^{-1-iz/2}\left[\int_0^\infty p^{-1}F(p)F(p/t)dp\right] dt \\ &= [\mathcal{M}(F \star G)]\,([z-i]/2) \\ &= [\mathcal{M}(F)]\,([z-i]/2)\,[\mathcal{M}(G)]\,([z-i]/2) \\ &= \frac{1}{2\pi}\tilde{F}(z/2)\tilde{F}(-z/2), \end{aligned}$$

where

$$\begin{aligned} \tilde{F}(z) &= \int_0^\infty x^{-1-iz} F(x) dx \\ &= \int_1^\infty x^{-1-iz} x^{-l/2}(x-1)^{-1/2} dx \\ &= \int_0^1 t^{l/2+iz-1/2}(1-t)^{-1/2} dt \\ &= \sqrt{\pi}\frac{\Gamma([l+1+2iz]/2)}{\Gamma([l+2+2iz]/2)}. \end{aligned}$$

The formula (1.5.22) follows.

The following pairs of Mellin transforms will be needed in Chapter 2, Section 2.2.3, and are easily verified by simple integration:

$$\psi^\sharp(s) = \frac{\mu^{-is}}{(s-ia)}, \quad \psi(p) = \begin{cases} i\sqrt{2\pi}\mu^a p^{-a-1/2}\theta(p-\mu) & \text{if } \mathrm{Re[a]} > 0 \\ -i\sqrt{2\pi}\mu^a p^{a-1/2}\theta(\mu-p) & \text{if } \mathrm{Re[a]} < 0. \end{cases} \tag{1.5.25}$$

1.6 Sobolev spaces

Let Ω be a non-empty, open subset of $\mathbb{R}^n$ with closure $\overline{\Omega}$ and boundary $\partial\Omega$. The norm in the Lebesgue space $L^p(\Omega),\ 1 \le p \le \infty$, is written

$$\|u\|_{p,\Omega} := \begin{cases} \left(\int_\Omega |u(\mathbf{x})|^p d\mathbf{x}\right)^{1/p}, & \text{if} \quad 1 \le \text{p} < \infty, \\ \text{ess sup}_{\mathbf{x}\in\mathbb{R}^3} |\text{u}(\mathbf{x})|, & \text{if} \quad \text{p} = \infty. \end{cases}$$

If there is no ambiguity we omit the subscript Ω and write $\|u\|_p$. In fact, in subsequent chapters, the underlying space is $L^2(\mathbb{R}^3)$ in which case we simply write $\|u\|$ for the norm. If the Lebesgue measure $d\mathbf{x}$ is replaced by a measure of the form $w(\mathbf{x})d\mathbf{x}$, we get the weighted space $L^p(\Omega; w(\mathbf{x})d\mathbf{x})$ with norm (when $1 \le p < \infty$)

$$\|u\|_{L^p(\Omega;w(\mathbf{x})d\mathbf{x})} := \left(\int_\Omega |u(\mathbf{x})|^p w(\mathbf{x}) d\mathbf{x}\right)^{1/p}.$$

We preserve this notation even for $L^p(\Omega)$ if there is the risk of confusion with different norms.

For points $\mathbf{x} = (x_1, x_2, \cdots, x_n) \in \mathbb{R}^n$ and n-tuples $\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_n) \in \mathbb{N}_0^n$, we write

$$|\mathbf{x}| = (\sum_{j=1}^n x_j^2)^{1/2},\ |\alpha| = \sum_{j=1}^n \alpha_j,\ D^\alpha = \prod_{j=1}^n D_j^{\alpha_j},$$

where $D_j = (1/i)\partial/\partial x_j$. For $k \in \mathbb{N}$ and $p \in [1, \infty]$, the *Sobolev space* $W^{k,p}(\Omega)$ is defined as

$$W^{k,p}(\Omega) := \{u : \Omega \to \mathbb{C}, u, D^\alpha u \in L^p(\Omega) \text{ for } |\alpha| \le k\},$$

where the derivatives $D^\alpha u$ are taken to be in the weak or distributional sense. It is endowed with the norm

$$\|u\|_{k,p,\Omega} := \begin{cases} \left(\sum_{0\le|\alpha|\le k} \|D^\alpha u\|_{p,\Omega}^p\right)^{1/p}, & \text{if } 1 \le p < \infty, \\ \sum_{0\le|\alpha|\le k} \|D^\alpha u\|_{\infty,\Omega}, & \text{if } p = \infty, \end{cases} \tag{1.6.1}$$

where $\|u\|_{p,\Omega}$ denotes the standard $L^p(\Omega)$ norm of u, namely $(\int_\Omega |u(\mathbf{x})|^p d\mathbf{x})^{1/p}$. $W^{k,p}(\Omega)$ is a separable Banach space if $p \in [1, \infty)$ and is reflexive if $p \in (1, \infty)$. When $p = 2, W^{k,2}(\Omega)$ is a Hilbert space with inner product

$$(u, v)_{k,2,\Omega} = \int_\Omega \sum_{|\alpha|\le k} D^\alpha u(\overline{D^\alpha v}) d\mathbf{x}.$$

When $\Omega = \mathbb{R}^n$, we shall omit Ω in the notation and write $\|\cdot\|_{k,p}$ and $(\cdot,\cdot)_{k,2}$.

Meyers and Serrin proved in [Meyers and Serrin (1964)] that for $p \in [1, \infty)$, $W^{k,p}(\Omega)$ coincides with the completion $H^{k,p}(\Omega)$ of the linear space $C^\infty(\Omega) \cap W^{k,p}(\Omega)$ with respect to $\|\cdot\|_{k,p,\Omega}$, i.e., $C^\infty(\Omega) \cap W^{k,p}(\Omega)$ is dense in $W^{k,p}(\Omega)$. As is now standard, we shall use the notation $H^k(\Omega)$ for $H^{k,2}(\Omega) \equiv W^{k,2}(\Omega)$.

We shall occasionally need the *Bessel potential spaces* $H^{s,p}(\mathbb{R}^n), s \in \mathbb{R}_+, p \in (1,\infty)$. These are defined in terms of the Bessel potential g_s, whose Fourier transform is given by

$$\hat{g}_s(\mathbf{p}) := (1+|\mathbf{p}|^2)^{-s/2};$$

see [Stein (1970)] for the properties of g_s. We have that

$$H^{s,p}(\mathbb{R}^n) := \{u : u = g_s * f \text{ for some } f \in L^p(\mathbb{R}^n)\} \tag{1.6.2}$$

with norm

$$\|u\|_{s,p} = \|f\|_p. \tag{1.6.3}$$

For all $s \geq 0$ and $p \in (1,\infty)$, the Schwartz space $\mathbf{S}(\mathbb{R}^\mathbf{n})$ is dense in $H^{s,p}(\mathbb{R}^n)$. When $s = k \in \mathbb{N}$, $H^{s,p}(\mathbb{R}^n)$ coincides with the Sobolev space $W^{k,p}(\mathbb{R}^n) \equiv H^{k,p}(\mathbb{R}^n)$. Since $\hat{f}(\mathbf{p}) = (1+|\mathbf{p}|^2)^{s/2}\hat{u}(\mathbf{p})$ if $u = g_s * f$, by (1.5.9), it follows from the Parseval formula (1.5.7) when $p = 2$ that

$$\|u\|_{s,2} = \left(\int_{\mathbb{R}^n} (1+|\mathbf{p}|^2)^s |\hat{u}(\mathbf{p})|^2 d\mathbf{p}\right)^{1/2}. \tag{1.6.4}$$

In particular, as $\mathbb{F}(D_j u)(\mathbf{p}) = p_j \hat{u}(\mathbf{p})$, by (1.5.5),

$$\|u\|_{1,2}^2 = \int_{\mathbb{R}^n} \left(|u(\mathbf{x})|^2 + |\nabla u(\mathbf{x})|^2\right) d\mathbf{x} \tag{1.6.5}$$

$$= \int_{\mathbb{R}^n} (1+|\mathbf{p}|^2)|\hat{u}(\mathbf{p})|^2 d\mathbf{p}, \tag{1.6.6}$$

where ∇ is the gradient and $|\nabla u|^2 = \sum_{j=1}^n |D_j u|^2$.

Important properties of the Sobolev and Bessel potential spaces are now listed; see [Edmunds and Evans (1987)], Chapter V, for proofs and further details. We shall assume that $p \in [1,\infty)$ unless otherwise stated.

(i) For $k \in \mathbb{R}$, $C_0^\infty(\mathbb{R}^n)$ is dense in $H^{k,p}(\mathbb{R}^n)$, and, for all $s \geq 0$, and $p \in (1,\infty)$, the Schwartz space $\mathbf{S}(\mathbb{R}^n)$ is dense in $H^{s,p}(\mathbb{R}^n)$.

(ii) The closure of $C_0^\infty(\Omega)$ in $H^{k,p}(\Omega)$ is denoted by $H_0^{k,p}(\Omega)$. Thus, by (i), $H^{k,p}(\mathbb{R}^n) = H_0^{k,p}(\mathbb{R}^n)$. If Ω is bounded, $H_0^{k,p}(\Omega) \neq H^{k,p}(\Omega)$. Also if Ω is bounded,

$$\|u\|_{p,\Omega} \leq \left(\frac{|\Omega|}{\omega_n}\right)^{1/n} \|\nabla u\|_{p,\Omega}, \quad \text{for all} \quad u \in H_0^{1,p}(\Omega), \tag{1.6.7}$$

where

$$\|\boldsymbol{\nabla} u\|_{p,\Omega} = \||\boldsymbol{\nabla} u|\|_{p,\Omega},$$

and $\omega_n = \pi^{n/2}/\Gamma(1+n/2)$ is the volume of the unit ball in $\mathbb{R}^n$. Hence

$$\|u\|_{1,p,\Omega} \lesssim \left(\sum_{|\alpha|=1} \|D^\alpha u\|_{p,\Omega}^p\right)^{1/p}.$$

It follows that the norm $\|\cdot\|_{1,p,\Omega}$ on $H_0^{1,p}(\Omega)$ is equivalent to the norm

$$\|u\|_{H_0^{1,p}(\Omega)} := \left(\sum_{|\alpha|=1} \|D^\alpha u\|_{p,\Omega}^p \right)^{1/p}. \tag{1.6.8}$$

(iii) Let $1 \le p < n$ and set $p^* = np/(n-p)$, the so-called *Sobolev conjugate* of p. Then the identification map is a continuous injection of $H_0^{1,p}(\Omega)$ into $L^{p^*}(\Omega)$: this continuous embedding is indicated by $H_0^{1,p}(\Omega) \hookrightarrow L^{p^*}(\Omega)$. This constitutes the case $1 \le p < n$ of the *Sobolev embedding theorem* for $H_0^1(\Omega)$.

(iv) For $1 \le p < n/k, H_0^{k,p}(\Omega)$ is continuously embedded in $L^s(\Omega)$, where $s = np/(n-kp)$.

(v) If $q \in [1, np/(n-kp))$ and Ω is bounded, $H_0^{k,p}(\Omega)$ is compactly embedded in $L^q(\Omega)$; this is the *Rellich–Kondrachov property.*

(vi) If Ω is bounded, $H_0^{1,n}(\Omega)$ is continuously embedded in the Orlicz space $L^\phi(\Omega)$, where $\phi(t) = \exp\left(t^{n/(n-1)} - 1\right), t \ge 0$, and, in particular, $H_0^{1,n}(\Omega) \hookrightarrow L^q(\Omega)$ for all $q \in [n, \infty)$. Note that $L^\phi(\Omega)$ is the linear span of the set of Lebesgue measurable functions u on Ω which are such that $\int_\Omega \phi(|u(\mathbf{x})|)d\mathbf{x} < \infty$, endowed with the norm

$$\|u\|_{L^\phi(\Omega)} := \inf\{\lambda : \int_\Omega \phi\left(\frac{|u(\mathbf{x})|}{\lambda}\right) d\mathbf{x} \le 1\}.$$

It is a Banach space containing $L^\infty(\Omega)$ which, in general, is neither reflexive nor separable.

(vii) If Ω is bounded and $p > n$, then $H_0^{1,p}(\Omega)$ is continuously embedded in the space $C^{0,\gamma}(\overline{\Omega})$ of functions u which are Hölder continuous on $\overline{\Omega}$ with exponent $\gamma = 1 - n/p$ and norm

$$\|u\|_{C^{0,\gamma}(\overline{\Omega})} := \|u\|_{L^\infty(\Omega)} + \sup_{\mathbf{x},\mathbf{y}\in\overline{\Omega},\mathbf{x}\ne\mathbf{y}} \frac{|u(\mathbf{x}) - u(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\gamma}.$$

The embedding of $H_0^{1,p}(\Omega)$ into $C^{0,\lambda}(\overline{\Omega})$ is compact for any $\lambda \in (0, \gamma)$.

(viii) If the boundary of Ω is sufficiently smooth (see [Edmunds and Evans (1987)], Section V.4) the above results in (iii)–(vii) continue to hold for $H^{k,p}(\Omega)$.

1.7 Inequalities

Three inequalities make regular appearances throughout the book, namely, the well-known inequalities of Sobolev, Hardy and Kato. We shall need only the L^2 versions of these inequalities, but mention some L^p versions for completeness.

- (Sobolev) For $1 \le p < n$, there exists a constant $C_{n,p}$, depending only on n and p, such that for all $f \in C_0^\infty(\mathbb{R}^n)$,

$$\|f\|_{p^*} \le C_{n,p}\|\nabla f\|_p = C_{n,p}\left(\int_{\mathbb{R}^n}[\sum_{j=1}^n |D_j u|^2]^{p/2} d\mathbf{x}\right)^{1/p}. \qquad (1.7.1)$$

The best possible value of the constant $C_{n,p}$ in (1.7.1) for $1 < p < n$ is

$$\pi^{-1/2} n^{-1/p}\left(\frac{p-1}{n-p}\right)^{(p-1)/p}\left\{\frac{\Gamma(1+n/2)\Gamma(n)}{\Gamma(n/p)\Gamma(1+n-n/p)}\right\}$$

and equality is attained for functions f of the form

$$f(\mathbf{x}) = [a + b|\mathbf{x}|^{p/(p-1)}]^{1-n/p},$$

where a and b are positive constants: these functions are obviously not in $C_0^\infty(\mathbb{R}^n)$ but lie in $L^p(\mathbb{R}^n)$ and the completion of $C_0^\infty(\mathbb{R}^n)$ with respect to the norm $\|\nabla \cdot\|_p$. When $p = 1$, $C_{n,1} = 1/n\omega_n^{1/n}$ is the optimal constant, and equality is never attained unless f vanishes identically. However, in this case the inequality has an extended version

$$\|f\|_{1^*} \le (n\omega_n^{1/n})^{-1}\|Df\|$$

on the set of functions f of bounded variation on $\mathbb{R}^n$, with Df the distributional gradient (a vector-valued Radon measure) and $\|Df\|$ the total variation of f in $\mathbb{R}^n$. For this inequality, the characteristic functions of arbitrary balls are extremals.

For $1 \le p < n$, (1.7.1) was established by Sobolev [Sobolev (1938)], the case $p = 1$ being later proved by Gagliardo [Gagliardo (1958)] and Nirenberg [Nirenberg (1959)]. The optimal constant for $p = 1$ was determined independently by Federer and Fleming in [Federer and Fleming (1960)] and Maz'ya in [Maz'ya (1960)], but for $p > 1$, the best constant was only found 10 years later, independently by Aubin [Aubin (1976)] and Talenti [Talenti (1976)].

- (Sobolev inequality for $\sqrt{-\Delta}$) For all $f \in \mathbf{S}(\mathbb{R}^n)$, $n \ge 2$ and $q = 2n/(n-1)$,

$$\|f\|_q^2 \le C_n \int_{\mathbb{R}^n} |\mathbf{p}||\hat{f}(\mathbf{p})|^2 d\mathbf{p}, \qquad (1.7.2)$$

where the optimal value of the constant C_n is

$$C_n = \left\{\left(\frac{n-1}{2}\right) 2^{1/n}\pi^{(n+1)/2n}\right\}^{-1}\Gamma\left(\frac{n+1}{2}\right)^{1/n}.$$

There is equality if and only if f is a constant multiple of a function of the form $[(\mu^2 + (\mathbf{x}-\mathbf{a})^2]^{-(n-1)/2}$ with $\mu > 0$ and $\mathbf{a} \in \mathbb{R}^n$ arbitrary. This is proved in [Lieb and Loss (1997)], Theorem 8.4.

- (Hardy) For all $f \in C_0^\infty(\mathbb{R}^n), n \geq 3$,

$$\int_{\mathbb{R}^n} \frac{|f(\mathbf{x})|^2}{|\mathbf{x}|^2} d\mathbf{x} \leq \left(\frac{2}{(n-2)}\right)^2 \int_{\mathbb{R}^n} |\boldsymbol{\nabla} f(\mathbf{x})|^2 d\mathbf{x}. \tag{1.7.3}$$

The constant is sharp and equality is only valid for $f = 0$. The inequality is determined by the radial part of $\boldsymbol{\nabla}$ and in fact

$$\int_{\mathbb{R}^n} \frac{|f(\mathbf{x})|^2}{|\mathbf{x}|^2} d\mathbf{x} \leq \left(\frac{2}{(n-2)}\right)^2 \int_{\mathbb{R}^n} |\frac{\partial}{\partial r} f(\mathbf{x})|^2 d\mathbf{x}. \tag{1.7.4}$$

By completion, (1.7.3) and (1.7.4) hold for all functions f which are such that ∇f or $(\partial/\partial r)f$ (in the weak, or distributional sense) lie in $L^2(\mathbb{R}^n)$. When $n = 2$, (1.7.3) is of course trivial, while when $n = 1$, we have that, for all f that are locally absolutely continuous on $(0, \infty)$, $f' \in L^2(0, \infty)$ and such that $\lim_{r\to 0+} f(r) = 0$,

$$\int_0^\infty \frac{|f(r)|^2}{r^2} dr \leq 4 \int_0^\infty |f'(r)|^2 dr. \tag{1.7.5}$$

The L^p version of the Hardy inequality is, for $1 \leq p < n$,

$$\int_{\mathbb{R}^n} \frac{|f(\mathbf{x})|^p}{|\mathbf{x}|^p} d\mathbf{x} \leq \left(\frac{p}{(n-p)}\right)^p \int_{\mathbb{R}^n} |\boldsymbol{\nabla} f(\mathbf{x})|^p d\mathbf{x}. \tag{1.7.6}$$

The constant is optimal and there are no non-trivial cases of equality.

- (Kato) For all $f \in \mathbf{S}(\mathbb{R}^n), n \geq 2$,

$$\int_{\mathbb{R}^n} \frac{|f\mathbf{x})|^2}{|\mathbf{x}|} d\mathbf{x} \leq c_n^2 \int_{\mathbb{R}^n} |\mathbf{p}||\hat{f}(\mathbf{p}|^2 d\mathbf{p}. \tag{1.7.7}$$

The best possible constant c_n for general values of $n \geq 2$ will be included in Theorem 1.7.1 below. In particular

$$c_3 = \sqrt{\pi/2}, \quad c_2 = \Gamma(1/4)/\sqrt{2}\Gamma(3/4).$$

There are no non-trivial cases of equality.

The above Hardy and Kato inequalities are special cases of the following inequality obtained by Herbst in [Herbst (1977)], Theorem 2.5. With $\mathbf{p} = -i\boldsymbol{\nabla}$ denoting the momentum operator, Herbst determines the norm of the operator $C_\alpha := |\mathbf{x}|^{-\alpha}|\mathbf{p}|^{-\alpha}$ as a map from $L^q(\mathbb{R}^n)$ into itself. The precise result is:

Theorem 1.7.1. *Let $\alpha > 0$ and $n\alpha^{-1} > q > 1$. Then C_α can be extended to a bounded operator from $L^q(\mathbb{R}^n)$ into itself, with norm*

$$\|C_\alpha : L^q(\mathbb{R}^n) \to L^q(\mathbb{R}^n)\| = \gamma(n, \alpha) := \frac{\Gamma(\frac{1}{2}[nq^{-1} - \alpha])\Gamma(\frac{1}{2}n(q')^{-1})}{2^\alpha \Gamma(\frac{1}{2}[n(q')^{-1} + \alpha])\Gamma(\frac{1}{2}nq^{-1})}, \tag{1.7.8}$$

where $q' = q/(q-1)$. If $q \geq n\alpha^{-1}$ or $q = 1$, C_α is unbounded.

In the case $q = 2$, $\mathbf{p}$ has adjoint $(1/i)$div and absolute value $|\mathbf{p}| = (\mathbf{p}^*\mathbf{p})^{1/2} = \sqrt{-\Delta}$. Also $|\mathbf{p}|$ is self-adjoint, injective and has dense range in $L^2(\mathbb{R}^n)$. Hence

$$\|C_\alpha\| = \sup_{\phi \in \mathcal{R}(|\mathbf{p}|^\alpha)} \frac{\|C_\alpha \phi\|_2}{\|\phi\|_2} = \sup_{\psi \in \mathcal{D}(|\mathbf{p}|^\alpha)} \frac{\||\mathbf{x}|^{-\alpha}\psi\|_2}{\||\mathbf{p}|^\alpha \psi\|_2},$$

where $\mathcal{R}, \mathcal{D}$ denote the range and domain respectively of the exhibited operator. Since $\mathbb{F}(|\mathbf{p}|^\alpha \psi)(\boldsymbol{\xi}) = |\boldsymbol{\xi}|^\alpha \hat{\psi}(\boldsymbol{\xi})$, it follows by Parseval's formula that (1.7.8) becomes

$$\int_{\mathbb{R}^n} \frac{1}{|\mathbf{x}|^{2\alpha}} |\psi(\mathbf{x})|^2 d\mathbf{x} \leq \gamma^2(n,\alpha) \int_{\mathbb{R}^n} |\boldsymbol{\xi}|^{2\alpha} |\hat{\psi}(\boldsymbol{\xi})|^2 d\boldsymbol{\xi},$$

which is Hardy's inequality in the case $\alpha = 1$ and Kato's inequality when $\alpha = 1/2$. In Section 2.2.1 we give an alternative proof to that of Herbst for the Kato inequality when $n = 2, 3$, using spherical harmonics.

Another inequality which features prominently throughout the book is the following generalisation of Hilbert's double series theorem due to Hardy, Littlewood and Pólya, see [Hardy *et al.* (1959)], Chapter IX, Section 319.

Theorem 1.7.2. *Let $K(\cdot,\cdot)$ be a non-negative function on $\mathbb{R}_+ \times \mathbb{R}_+$ that is homogeneous of degree -1, i.e., for any $\lambda \in \mathbb{R}_+, K(\lambda x, \lambda y) = \lambda^{-1} K(x,y)$. Suppose also that for $p > 1$, we have*

$$\int_0^\infty K(x,1) x^{-1/p} dx = \int_0^\infty K(1,y) y^{-1/p'} dy = k, \tag{1.7.9}$$

where $p' = p/(p-1)$. Then

$$\int_0^\infty \int_0^\infty K(x,y)|f(x)g(y)| dx dy \leq k \left(\int_0^\infty |f(x)|^p dx \right)^{1/p} \left(\int_0^\infty |g(y)|^{p'} dy \right)^{1/p'}, \tag{1.7.10}$$

$$\int_0^\infty dy \left(\int_0^\infty K(x,y)|f(x)| dx \right)^p \leq k^p \int_0^\infty |f(x)|^p dx, \tag{1.7.11}$$

$$\int_0^\infty dx \left(\int_0^\infty K(x,y)|g(y)| dy \right)^{p'} \leq k^{p'} \int_0^\infty |g(y)|^{p'} dy. \tag{1.7.12}$$

If $K(\cdot,\cdot)$ is positive, then there is inequality in (1.7.11) unless $f = 0$, in (1.7.12) unless $g = 0$, and in (1.7.10) unless either $f = 0$ or $g = 0$.

1.8 CLR and related inequalities

The CLR refers to Cwikel–Lieb–Rosenbljum who proved the inequality independently and by very different methods in [Cwikel (1977)], [Lieb (1976)] and [Rozenbljum (1972)]. The names are listed alphabetically, but in reverse chronological order of discovery. In its original form, the inequality concerns the self-adjoint operator $-\Delta - V$ defined as a form sum, whose spectrum is discrete below 0 and with V the operator of multiplication by a function V with a positive part $V_+ := (1/2)(|V|+V) \in L^{n/2}(\mathbb{R}^n)$. It asserts that, for $n \geq 3$, the number $N(-\Delta - V)$ of negative eigenvalues of $-\Delta - V$ satisfies

$$N(-\Delta - V) \leq c(n) \int_{\mathbb{R}^n} V_+(\mathbf{x})^{n/2} d\beta x, \tag{1.8.1}$$

for some constant $c(n)$ depending only on n. Other proofs have also been given, notably those of Li and Yau [Li and Yau (1983)] and Conlon [Conlon (1984)]. A treatment, which is particularly suitable for our needs, is that given by Rozenbljum and Solomyak in [Rozenbljum and Solomyak (1998)]. This is motivated by Lieb's proof and gives an abstract version of the inequality, which can be applied to other operators that feature in the book.

In order to state the main results in [Rozenbljum and Solomyak (1998)] it is necessary to recall some basic facts about the operator semigroup $e^{-tT}, 0 \leq t < \infty$, associated with a non-negative, self-adjoint operator T acting in a Hilbert space H.

(1) $Q(t) := e^{-tT}, 0 \leq t < \infty$, is *strongly continuous*, i.e.

$$\lim_{t \to s} \|Q(t)f - Q(s)f\| = 0, \quad \text{for all} \quad f \in H,$$

and *contractive*, i.e.

$$\|Q(t)f\| \leq \|f\|, \quad \text{for all} \quad f \in H.$$

(2) T is the *infinitesimal generator* of $Q(t)$, i.e.

$$Tf = \lim_{t \to 0+} \frac{1}{t}\{f - Q(t)f\}, \quad \text{for all} \quad f \in \mathcal{D}(T).$$

(3) For $f \in \mathcal{D}(T), Q(t)f \in \mathcal{D}(T)$ and

$$\frac{\partial}{\partial t}[Q(t)f] := \lim_{\varepsilon \to 0} \left\{ \frac{1}{\varepsilon}[Q(t+\varepsilon) - Q(t)]f \right\} = -TQ(t)f = -Q(t)Tf, \quad (t > 0),$$
$$Q(0)f := \lim_{t \to 0+} Q(t)f = f.$$

The result in [Rozenbljum and Solomyak (1998)] deals with the set $\mathcal{P}$ of positive, self-adjoint operators in a space $L^2(\Omega)$ say, which are positivity preserving and have the $(2, \infty)$ mapping property. An operator B is *positivity preserving* (or its associated semi-group $\mathcal{Q}_B(t) := e^{-tB}, 0 \leq t < \infty$, is *positivity preserving*) if $\mathcal{Q}_B(t)u \geq 0$ for all non-negative functions $u \in L^2(\Omega)$. It has the $(2, \infty)$ *mapping property* if $\mathcal{Q}_B(t) : L^2(\Omega) \to L^\infty(\Omega)$ is bounded: for Markov semigroups, the $(2, \infty)$ property is usually called *ultracontractivity*. Semigroups which are positivity preserving and have the $(2, \infty)$ property are known to be integral operators. The kernel $Q_B(t; x, y)$ of $\mathcal{Q}_B(t)$ satisfies the symmetry condition $Q_B(t; x, y) = \overline{Q_B(t; y, x)}$ and it follows from the fact that $\mathcal{Q}_B(t)$ is a semigroup that, for a.e. $x \in \Omega$,

$$Q_B(t; x, x) = \int_\Omega Q_B(t_1; x, y) Q_B(t_2; x, y) dy, \quad t_1, t_2 > 0, \; t = t_1 + t_2$$

is well defined as an element of $L^\infty(\Omega)$, which does not depend on the particular choice of t_1 and t_2. Moreover,

$$\begin{aligned} M_B(t) := \|e^{-tB} : L^2 \to L^\infty\| &= \mathrm{esssup}_{x\in\Omega} \int |Q_B(t/2;x,y)|^2 dy < \infty. \\ &= \mathrm{esssup}_{x\in\Omega} \int Q_B(t/2;x,y) Q_B(t/2;y,x) dy \\ &= \mathrm{esssup}_{x\in\Omega} Q_B(t;x,x). \end{aligned}$$

For $B \in \mathcal{P}$, the kernel $Q_B(t;x,y)$ is non-negative, a.e. on $\mathbb{R}_+ \times \Omega \times \Omega$. If $B \in \mathcal{P}$, and $B \geq c$ for some $c \geq 0$, then, for any $r \geq -c, B_r := B + r \in \mathcal{P}, \mathcal{Q}_{B_r}(t) = e^{-rt}\mathcal{Q}_B(t)$ and $M_{B_r} = e^{-rt} M_B(t)$.

The following is Theorem 2.1 in [Rozenbljum and Solomyak (1998)] and is given in terms of a non-negative, convex function G on $[0,\infty)$ which grows polynomially at infinity and is such that $G(z) = 0$ near $z = 0$. Let

$$g(r) := \int_0^\infty z^{-1} G(z) e^{-z/r} dz.$$

In the theorem, multiplication by V is assumed to be such that self-adjoint operators $B - V$ and $A - V$ can be defined as form sums; see Section 1.2.

Theorem 1.8.1. *Let $B \in \mathcal{P}$ be such that $M_B \in L^1(a,\infty)$, $a > 0$ and $M_B(t) = O(t^{-\alpha})$ at zero for some $\alpha > 0$. Then, in the above notation,*

$$N(B - V) \leq \frac{1}{g(1)} \int_0^\infty \frac{dt}{t} \int_\Omega M_B(t) G[tV_+(x)] dx. \tag{1.8.2}$$

The inequality continues to hold for $N(A - V)$ when A is a non-negative, self-adjoint operator, which is such that e^{-tA} is dominated by a positivity preserving semigroup e^{-tB} in the sense that

$$|e^{-tA}\psi| \leq e^{-tB}|\psi| \quad \text{a.e. } on \quad \Omega. \tag{1.8.3}$$

We denote the class of such operators A by $\mathcal{PD}(B)$.

If $A \in \mathcal{PD}(B)$ then $A + r \in \mathcal{PD}(B + r)$. Also, a particular result from [Bratelli *et al.* (1980)] is that if e^{-tB} is positivity preserving and $A \in \mathcal{PD}(B)$, then for $0 < \alpha < 1$, e^{-tB^α} is positivity preserving and $A^\alpha \in \mathcal{PD}(B^\alpha)$. Any $A \in \mathcal{PD}(B)$ is an integral operator and (1.8.3) is equivalent to

$$|Q_A(t;x,y)| \leq Q_B(t;x,y) \quad \text{a.e.} \quad \text{on} \quad \mathbb{R}_+ \times \Omega \times \Omega. \tag{1.8.4}$$

We refer to [Rozenbljum and Solomyak (1998)] for details and full references. Of particular interest to us are the following examples discussed in [Rozenbljum and Solomyak (1998)], which are special cases of Theorem 1.8.1. In all cases $\Omega = \mathbb{R}^n$.

1.8.1 *The Schrödinger operator*

The semigroup associated with the Laplace operator $B := -\Delta$ is the heat operator, which is an integral operator with kernel

$$Q_B(t;\mathbf{x},\mathbf{y}) = \frac{1}{(4\pi t)^{n/2}} \exp\left\{\frac{-|\mathbf{x}-\mathbf{y}|^2}{4t}\right\}. \tag{1.8.5}$$

Thus $Q_B(t)$ is positivity preserving. Furthermore, an application of the Cauchy–Schwarz inequality readily yields

$$\|Q_B(t)f\|_{L^\infty(\mathbb{R}^n)} \le 2^{-n}\|f\|_{L^2(\mathbb{R}^n)}$$

and so $Q_B(t)$ has the $(2,\infty)$ property. Consequently $B = -\Delta \in \mathcal{P}$ and $M_B(t) = \frac{1}{(4\pi t)^{n/2}}$, so that $M_B \in L^1(a,\infty), a > 0$, if and only if $n \ge 3$. Hence, to apply Theorem 1.8.1 we need $n \ge 3$.

Following Lieb in [Lieb (1976)], the choice $G(z) = (z-a)_+$ in (1.8.1), where $(\cdot)_+$ denotes the positive part and a is a positive constant to be chosen, yields

$$N(-\Delta - V) \le C(G)\int_{\mathbb{R}^n} V_+^{n/2}(\mathbf{x})d\mathbf{x}, \tag{1.8.6}$$

where $C(G) = (2\pi)^{-n/2}g(1)^{-1}\int_a^\infty (t-a)t^{-n/2-1}dt$. The optimal value of $C(G)$ as a function of a is .1156, attained when $a = 1/4$. This coincides with Lieb's constant in [Lieb (1976)], which is the best value achieved to date.

1.8.2 *The magnetic Schrödinger operator*

This is of the form $-\Delta_{\mathbf{A}} - V$, where $\Delta_{\mathbf{A}}$ is the *magnetic Laplacian*

$$\Delta_{\mathbf{A}} = (\boldsymbol{\nabla} + i\mathbf{A})^2 = \sum_{j=1}^n (\partial_j + iA_j)^2,$$

and $\mathbf{A} = \{A_j : j = 1,\cdots,n\}$ is the magnetic potential. A number of proofs exist of the result that $A \in \mathcal{PD}(-\Delta)$; see the discussion and a list of references after Theorem 2.3 in [Avron *et al.* (1978)]. It then follows from Theorem 1.8.1 that

$$N(-\Delta_{\mathbf{A}} - V) \le C(G)\int_{\mathbb{R}^n} V_+^{n/2}(\mathbf{x})d\mathbf{x}, \tag{1.8.7}$$

with the same constant as in (1.8.6). It is not true in general that $N(-\Delta_{\mathbf{A}} - V) \le N(-\Delta - V)$; see [Avron *et al.* (1978)], Example 2 following Theorem 2.14.

1.8.3 *The quasi-relativistic Schrödinger operator*

The pseudo-differential operator $B = \sqrt{-\Delta}$ is non-negative and self-adjoint, with domain $H^1(\mathbb{R}^n)$. The kernel of the associated semigroup $Q_B(t)$ is the Poisson kernel

$$\begin{aligned} Q_B(t;\mathbf{x},\mathbf{y}) &= \int_{\mathbb{R}^n} \exp[-2\pi|\mathbf{k}|t + 2\pi i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})]d\mathbf{k} \\ &= \Gamma\left(\frac{n+1}{2}\right)\pi^{-(n+1)/2}\frac{t}{[t^2+|\mathbf{x}-\mathbf{y}|^2]^{(n+1)/2}}; \end{aligned}$$

see [Stein and Weiss (1971)], Theorem 1.14, and [Lieb and Loss (1997)], Section 7.11. Thus,

$$\|Q_B(t)f\|_{L^\infty(\mathbb{R}^n)} \le c_n \sup_{\mathbf{x}\in\mathbb{R}^n} \left(\int_{\mathbb{R}^n} \frac{t^2}{[t^2+|\mathbf{x}-\mathbf{y}|^2]^{(n+1)}} d\mathbf{y} \right)^{1/2} \|f\|_{L^2(\mathbb{R}^n)}$$
$$< c_n(t)\|f\|_{L^2(\mathbb{R}^n)}$$

for a positive constant $c_n(t)$ which is finite for all $t > 0$. Thus $B = \sqrt{-\Delta}$ has the $(2,\infty)$ property and lies in $\mathcal{P}$, with $M_B(t) = c_n t^{-n}$. Theorem 1.8.1 therefore applies for all $n \ge 2$ and leads to *Daubechies' inequality*

$$N(\sqrt{-\Delta} - V) \le C_n(G) \int_{\mathbb{R}^n} V_+(\mathbf{x})^n d\mathbf{x}, \tag{1.8.8}$$

where in the above notation and the same choice of G, $C_n(G) = g(1)^{-1} \int_0^\infty t^{-n-1} G(t) dt$.

The pseudo-differential operator $\mathbb{H}_0 = \sqrt{-\Delta+1}$, is self-adjoint with domain $H^1(\mathbb{R}^n)$ and $\mathbb{H}_0 \ge 1$. It will feature prominently throughout the book. From the result in [Bratelli *et al.* (1980)] noted above, it follows that with $B := \mathbb{H}_0 - 1, e^{-tB}$ is positivity preserving. It is an integral operator and on the diagonal, the kernel is given by

$$Q_B(t;\mathbf{x},\mathbf{x}) = (2\pi)^{n/2} \int_{\mathbb{R}^n} e^{-t[(|\xi|^2+1)^{1/2}-1]} d\xi, \tag{1.8.9}$$

from which we can easily infer that $e^{-t[\mathbb{H}_0-1]}$ has the $(2,\infty)$ property and

$$M_B(t) \le C(t^{-n/2} + t^{-n}).$$

For $n \ge 3$, Theorem 1.8.1 yields Daubechies' inequality

$$N(\mathbb{H}_0 - 1 - V) \le C_n(G) \int_{\mathbb{R}^n} V_+(\mathbf{x})^n d\mathbf{x} + C_{n/2}(G) \int_{\mathbb{R}^n} V_+(\mathbf{x})^{n/2} d\mathbf{x}, \tag{1.8.10}$$

where, in the above notation and the same choice of G, $C_a(G) = g(1)^{-1} \int_0^\infty t^{-a-1} G(t) dt$.

1.8.4 *The magnetic quasi-relativistic Schrödinger operator*

The operator $\sqrt{-\Delta_{\mathbf{A}}}$ lies in $\mathcal{PD}(-\Delta_{\mathbf{A}})$ by the result from [Bratelli *et al.* (1980)] quoted above and also satisfies (1.8.8):

$$N(\sqrt{-\Delta_{\mathbf{A}}} - V) \le C_n(G) \int_{\mathbb{R}^n} V_+(\mathbf{x})^n d\mathbf{x}. \tag{1.8.11}$$

Similarly,

$$N([(-\Delta_{\mathbf{A}}+1)^{1/2} - 1] - V) \le C_n(G) \int_{\mathbb{R}^n} V_+(\mathbf{x})^n d\mathbf{x} + C_{n/2}(G) \int_{\mathbb{R}^n} V_+(\mathbf{x})^{n/2} d\mathbf{x}. \tag{1.8.12}$$

1.9 Lieb–Thirring inequalities

These inequalities have a pivotal role in problems such as the stability of many-body systems composed of fermions. In many cases, the Hamiltonian describing the system is bounded below in terms of the sum of the negative eigenvalues of a one-body Hamiltonian. We shall see examples of this in Section 4.5 of Chapter 4. Since the seminal papers [Lieb and Thirring (1975)] and [Lieb and Thirring (1976)], Lieb–Thirring inequalities have come to mean estimates for moments of the negative eigenvalues of operators of Schrödinger type in terms of external electric and magnetic fields. The original result proved by Lieb and Thirring in [Lieb and Thirring (1975)], is that if $\gamma > \max\ (0, 1 - \mathrm{n}/2)$, then there exists a universal constant $L_{\gamma,n}$ such that

$$\sum_{n\in\mathbb{N}} |\lambda_j(S)|^\gamma \leq L_{\gamma,n} \int_{\mathbb{R}^n} V_+(\mathbf{x})^{\gamma+n/2} d\mathbf{x}, \tag{1.9.1}$$

where $\lambda_1(S) \leq \lambda_2(S) \leq \cdots$ are the negative eigenvalues of the Schrödinger operator $S := -\Delta - V$ counting multiplicities: the assumptions on V imply that the negative spectrum of S is discrete and its essential spectrum fills the positive half-line. Note that the case $n \geq 3, \gamma = 0$ is the CLR inequality associated with $-\Delta - V$.

If $V \in L^{\gamma+n/2}(\mathbb{R}^n)$, one has the Weyl-type asymptotic formula

$$\begin{aligned}\lim_{\alpha\to\infty} \alpha^{-(\gamma+n/2)} \sum_{n\in\mathbb{N}} |\lambda_j(S_\alpha)|^\gamma &= (2\pi)^{-n} \lim_{\alpha\to\infty} \alpha^{-(\gamma+n/2)} \int\int_{\mathbb{R}^n\times\mathbb{R}^n} (|\boldsymbol{\xi}|^2 - \alpha V)_+^\gamma d\mathbf{x} d\boldsymbol{\xi} \\ &= L_{\gamma,n}^{cl} \int_{\mathbb{R}^n} V_+(\mathbf{x})^{\gamma+n/2} d\mathbf{x},\end{aligned} \tag{1.9.2}$$

where $S_\alpha : -\Delta - \alpha V$ and the so-called classical constant $L_{\gamma,n}^{cl}$ is given by

$$L_{\gamma,n}^{cl} = (2\pi)^{-n} \int_{\mathbb{R}^n} (|\boldsymbol{\xi}| - 1)_+^\gamma d\boldsymbol{\xi} = \frac{\Gamma(\gamma+1)}{2^n \pi^{n/2} \Gamma(\gamma + n/2 + 1)}.$$

Therefore

$$L_{\gamma,n}^{cl} \leq L_{\gamma,n}.$$

The precise value of $L_{\gamma,n}$ is unknown in general, but a great deal is known in special cases. We refer to [Hundertmark *et al.* (2000)] for an up to date account.

The inequality (1.9.1) remains valid if a magnetic potential $\mathbf{A} = (A_1, \cdots, A_n), A_j \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$ for $j = 1, \cdots, n$, is introduced. That is, with

$$S(\mathbf{A}) := (i\nabla + \mathbf{A})^2 - V = \sum_{j=1}^n (i\partial_j + A_j)^2 - V$$

we have

$$\sum_{n\in\mathbb{N}} |\lambda_j(S(\mathbf{A}))|^\gamma \leq L_{\gamma,n} \int_{\mathbb{R}^n} V_+(\mathbf{x})^{\gamma+n/2} d\mathbf{x}, \tag{1.9.3}$$