Analytic criteria in the qualitative spectral analysis of the Schrödinger operator *

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Dedicated to Barry Simon on the occasion of his 60th birthday

Abstract. A number of topics in the qualitative spectral analysis of the Schrödinger operator $-\Delta+V$ are surveyed. In particular, some old and new results concerning the positivity and semiboundedness of this operator as well as the structure of different parts of its spectrum are considered. The attention is focused on conditions both necessary and sufficient, as well as on their sharp corollaries.

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1 Introduction

The purpose of the present article is to survey various analytic results concerning the Schrödinger operator $-\Delta + V(x)$ obtained during the last half-century, including several quite recently. In particular, the positivity and semiboundedness of this operator as well as the structure of different parts of its spectrum are among the topics touched upon.

In the choice of material I aim mostly at results of final character, i.e. at simultaneously necessary and sufficient conditions, and their consequences, the best possible in a sense. Another motivation for the inclusion of any particular problem in this survey is my own involvement in its solution.

Naturally, the selection of topics is far from exhaustive. For instance, conditions for the essential self-adjointness of the Schrödinger operator and for the absence of eigenvalues at positive energies, as well as properties of eigenfunctions and bounds on the number of eigenvalues, are not considered here. These and many other themes of qualitative spectral analysis have been discussed in the comprehensive surveys [Sim4], [BMS], [Dav1], and, of course, in the classical Reed and Simon's treatise [RS1]-[RS4]. However, the information collected in what follows has been quoted rarely if ever in the quantum mechanics literature.

Due to space limitation, I write only about the linear Schrödinger operator with electric potential, although some of the results below can be modified and applied to nonlinear, magnetic, relativistic Schrödinger operators and even general elliptic operators with variable coefficients. For the same reason, proofs are supplied just in a few cases, mostly when a source does not seem readily available.

2 Wiener capacity

The capacity of a set in $\mathbb{R}^n$ will be met frequently in the present article. This notion appeared first in electrostatics and was introduced to mathematics by N. Wiener in the 1920s. Since then several generalizations and modifications of Wiener's capacity appeared: Riesz, Bessel, polyharmonic capacities, p-capacity and others. They are of use in potential theory, probability, function theory and partial differential equations. The capacities provide adequate terms to describe sets of discontinuities of Sobolev functions, removable singularities of solutions to partial differential equations, sets of uniqueness for analytic functions, regular boundary points in the Wiener sense, divergence sets for trigonometric series, etc. (see, for example, [AH], [Car], [Lan], [MH]). Some applications of Wiener's and other capacities to the theory of the Schrödinger operator are presented in this survey.

Let Ω be an open set in $\mathbb{R}^n$ and let F be a compact subset of Ω. The Wiener (harmonic) capacity of F with respect to Ω is defined as the number

$$\mathrm{cap}_\Omega F = \inf\Big\{\int_\Omega |\nabla u|^2 dx : \ u \in C_0^\infty(\Omega), \ u \ge 1 \text{ on } F\Big\}. \tag{1}$$

We shall use the simplified notation $\mathrm{cap}F$ if $\Omega = \mathbb{R}^n$. The capacity $\mathrm{cap}_\Omega F$ can be defined equivalently as the least upper bound of $\nu(F)$ over the set of all measures ν supported by F and satisfying the condition

$$\int_\Omega G(x, y)\, d\nu(y) \le 1,$$

where G is the Green function of the domain Ω. If $\Omega = \mathbb{R}^3$ then it is just the electrostatic capacity of F.

It follows from the definition (1) that the capacity is a nondecreasing function of F and a nonincreasing one of Ω. We have Choquet's inequality

$$\operatorname{cap}_\Omega(F_1 \cap F_2) + \operatorname{cap}_\Omega(F_1 \cup F_2) \le \operatorname{cap}_\Omega F_1 + \operatorname{cap}_\Omega F_2$$

for arbitrary compact sets F_1 and F_2 in Ω [Cho]. It is easy to check that the Wiener capacity is continuous from the right. This means that for each $\varepsilon > 0$ there exists a neighborhood G, $F \subset G \subset \overline{G} \subset \Omega$ such that for each compact set F_1 with $F \subset F_1 \subset G$ the inequality

$$\operatorname{cap}_\Omega F_1 \le \operatorname{cap}_\Omega F + \varepsilon$$

holds.

Let E be an arbitrary subset of Ω. The inner and the outer capacities are defined as numbers

$$\underline{\operatorname{cap}}_\Omega E = \sup_{F \subset E} \operatorname{cap}_\Omega F, \qquad F \text{ compact in } \Omega,$$

$$\overline{\operatorname{cap}}_\Omega E = \inf_{G \supset E} \operatorname{cap}_\Omega G, \qquad G \text{ open in } \Omega.$$

It follows from the general Choquet theory that for each Borel set both capacities coincide [Cho]. Their common value is called the Wiener (harmonic) capacity and will be denoted by $\operatorname{cap}_\Omega E$.

By v_n we denote the volume of the unit ball in $\mathbb{R}^n$ and let $\operatorname{mes}_n F$ stand for the n-dimensional Lebesgue measure of F. By the classical isoperimetric inequality, the following isocapacitary inequalities hold (see [Maz7], Sect. 2.2.3)

$$\operatorname{cap}_\Omega F \ge n v_n^{2/n}(n-2)\,|(\operatorname{mes}_n \Omega)^{(2-n)/n} - (\operatorname{mes}_n F)^{(2-n)/n}|^{-1} \quad \text{if } n > 2 \qquad (2)$$

and

$$\operatorname{cap}_\Omega F \ge 4\pi \Big(\log \frac{\operatorname{mes}_2 \Omega}{\operatorname{mes}_2 F}\Big)^{-1} \quad \text{if } n = 2. \qquad (3)$$

In particular, if $n > 2$ then

$$\operatorname{cap} F \ge n v_n^{2/n}(n-2)(\operatorname{mes}_n F)^{(n-2)/n}. \qquad (4)$$

If Ω and F are concentric balls, then the three preceding estimates come as identities.

Using Wiener's capacity, one can obtain two-sided estimates for the best constant in the Friedrichs inequality

$$\|u\|_{L_2(B_1)} \le C\,\|\nabla u\|_{L_2(B_1)}, \qquad (5)$$

where B_1 is a unit open ball and u is an arbitrary function in $C^\infty(\overline{B_1})$ vanishing on a compact subset F of $\overline{B_1}$.

Proposition 2.1 [Maz2] *The best constant C in* (5) *satisfies*

$$C \le c(n)\big(\operatorname{cap} F\big)^{-1/2}, \qquad (6)$$

where $c(n)$ depends only on n.

It is shown in [MShu2] that (6) holds with $c(n) = 4 v_n n^{-1}(n^2-2)$. Proposition 2.1 has the following partial converse.

Proposition 2.2 *Let*

$$\operatorname{cap} F \leq \gamma \operatorname{cap} B_1, \tag{7}$$

where $\gamma \in (0,1)$. *Then any constant* C *in* (5) *satisfies*

$$C \geq c(n,\gamma)\big(\operatorname{cap} F\big)^{-1/2}. \tag{8}$$

This assertion was proved in [Maz2] (see also [Maz7], Ch. 10) with a sufficiently small $\gamma = \gamma(n)$. The present stronger version is essentially contained in [MShu1]. Both propositions were used in [KMS] to derive a discreteness of spectrum criterion for the magnetic Schrödinger operator.

3 Equality of the minimal and maximal Dirichlet Schrödinger forms

Let $\mathbb{V}$ be a nonnegative Radon measure in Ω. Consider the quadratic form

$$Q[u,u] = \int_\Omega |\nabla u|^2\, dx + \int_\Omega |u|^2\, \mathbb{V}(dx). \tag{9}$$

The closure of Q defined on the set

$$\{u \in C^\infty(\mathbb{R}^n) : \operatorname{supp} u \subset \Omega,\ Q[u,u] < \infty\},$$

which may contain functions with non-compact support, will be denoted by $Q_{\max}$. Another quadratic form $Q_{\min}$ is introduced as the closure of Q defined on $C_0^\infty(\Omega)$.

The question as to when the equality $Q_{\max} = Q_{\min}$ holds has been raised by T. Kato [Ka3]. B. Simon studied a similar question concerning the magnetic Schrödinger operator in $\mathbb{R}^n$ [Sim2]. The following necessary and sufficient condition for this equality was obtained in [CMaz].

Theorem 3.1 (i) *If either* $n \leq 2$ *or* $n > 2$ *and* $\operatorname{cap}(\mathbb{R}^n \backslash \Omega) = \infty$, *then* $Q_{\max} = Q_{\min}$.

(ii) *Suppose that* $n > 2$ *and* $\operatorname{cap}(\mathbb{R}^n \backslash \Omega) < \infty$. *Then* $Q_{\max} = Q_{\min}$ *if and only if*

$$\mathbb{V}(\Omega \backslash F) = \infty \quad \text{for every closed set } F \subset \Omega \text{ with } \operatorname{cap} F < \infty. \tag{10}$$

Example. Consider the domain Ω complementing the infinite funnel

$$\{x = (x', x_n) : x_n \geq 0,\ |x'| \leq f(x_n)\},$$

where f is a continuously decreasing function on $[0,\infty)$ subject to $f(t) \leq c f(2t)$. One can show that $\operatorname{cap}(\mathbb{R}^n \backslash \Omega) < \infty$ if and only if the function $f(t)^{n-2}$ for $n > 3$ and the function $(\log(t/f(t)))^{-1}$ for $n = 3$ are integrable on $(1,\infty)$.

Remark 3.1 Note that the equality $Q_{\max} = Q_{\min}$ is equivalent to (10) in the particular case $\Omega = \mathbb{R}^n$. Assume that $\mathbb{V}(dx) = V(x)\, dx$, where V is a positive function in $L^1_{\text{loc}}(\mathbb{R}^n)$ locally bounded away from zero. According to [CMaz], condition (10) is necessary for the essential self-adjointness of the operator $V^{-1}\Delta$ on $L^2(V\, dx)$ with domain $C_0^\infty(\mathbb{R}^n)$.

4 Closability of quadratic forms

Let Ω be an open set in $\mathbb{R}^n$ and let $\mathbb{V}$ be a nonnegative Radon measure in Ω. By $\mathring{L}_2^1(\Omega)$ we denote the completion of $C_0^\infty(\Omega)$ in the norm $\|\nabla u\|_{L_2(\Omega)}$.

One says that the quadratic form

$$\|u\|^2_{L_2(\Omega,\mathbb{V}(dx))} := \int_\Omega |u|^2\, \mathbb{V}(dx) \tag{11}$$

defined on $C_0^\infty(\Omega)$ is closable in $\mathring{L}_2^1(\Omega)$ if any Cauchy sequence in the space $L_2(\Omega, \mathbb{V}(dx))$ converging to zero in $\mathring{L}_2^1(\Omega)$ has zero limit in $L_2(\Omega, \mathbb{V}(dx))$. We call the measure $\mathbb{V}$ absolutely continuous with respect to the harmonic capacity if the equality $\operatorname{cap} E = 0$, where E is a Borel subset of Ω, implies $\mathbb{V}(E) = 0$. $\square$

Let, for example, $\mathbb{V}$ be the φ-Hausdorff measure in $\mathbb{R}^n$, i.e.

$$\mathbb{V}(E) = \lim_{\varepsilon\to+0} \inf_{\{\mathcal{B}^{(j)}\}} \sum_i \varphi(r_i),$$

where φ is a nondecreasing positive continuous function on $(0,\infty)$ and $\{\mathcal{B}^{(j)}\}$ is any covering of the set E by open balls $\mathcal{B}^{(i)}$ with radii $r_i < \varepsilon$. It is well known that this measure is absolutely continuous with respect to the Wiener capacity if

$$\int_0^\infty \varphi(t)\, t^{1-n}\, dt < \infty,$$

and that this condition is sharp in a sense (see [Car]).

Needless to say, any measure $\mathbb{V}$ absolutely continuous with respect to the n-dimensional Lebesgue measure is absolutely continuous with respect to the capacity. $\square$

The following result has been obtained in [Maz3].

Theorem 4.1 *The quadratic form (11) is closable in $\mathring{L}_2^1(\Omega)$ if and only if $\mathbb{V}$ is absolutely continuous with respect to the Wiener capacity.*

The closability of (11) in $\mathring{L}_2^1(\Omega)$ is necessary for the Schrödinger operator $-\Delta - \mathbb{V}$, formally associated with the form

$$S[u,u] := \int_\Omega |\nabla u|^2\, dx - \int_\Omega |u|^2\, \mathbb{V}(dx), \quad u \in C_0^\infty(\Omega), \tag{12}$$

to be well-defined. $\square$

Dealing with the Schrödinger operator formally given by the expression $-\Delta + \mathbb{V}$ and acting in $L_2(\Omega)$ we need the following notion of a form closable in $L_2(\Omega)$.

By definition, the quadratic form Q defined on $C_0^\infty(\Omega)$ by (9) is closable in $L_2(\Omega)$ if any Cauchy sequence in the norm $Q[u,u]^{1/2}$ which tends to zero in $L_2(\Omega)$ has zero limit in the norm $Q[u,u]^{1/2}$. This notion is equivalent to the lower semicontinuity of Q in $L_2(\Omega)$ [Sim1].

Theorem 4.2 (see[Maz7], Sect. 12.4, 12.5) *The form Q defined on $C_0^\infty(\Omega)$ is closable in $L_2(\Omega)$ if and only if $\mathbb{V}$ is absolutely continuous with respect to the Wiener capacity.*

We assume in the sequel that the measure $\mathbb{V}$ is absolutely continuous with respect to the Wiener capacity.

5 Positivity of the Schrödinger operator with negative potential

The next result was obtained in [Maz1], [Maz3] (see also [Maz7], Th. 2.5.2).

Theorem 5.1 *Let Ω be an open set in $\mathbb{R}^n$, $n \geq 1$, and let $\mathbb{V}$ be a nonnegative Radon measure in Ω. The inequality*

$$\int_\Omega |u|^2\, \mathbb{V}(dx) \leq \int_\Omega |\nabla u|^2\, dx \tag{13}$$

holds for every $u \in C_0^\infty(\Omega)$ provided

$$\frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} \leq \frac{1}{4} \tag{14}$$

for all compact sets $F \subset \Omega$.

A necessary condition for (13) is

$$\frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} \leq 1, \tag{15}$$

where F is an arbitrary compact subset of Ω.

Remark 5.1 In inequalities (14), (15) and elsewhere in similar cases, we tacitly assume that vanishing of denominator implies vanishing of numerator, and we may choose any appropriate value of the ratio.

Remark 5.2 The necessity of (15) is trivial. The proof of sufficiency of (14) in [Maz3], [Maz7] shows that (14) implies (13) even without the requirement $\mathbb{V} \geq 0$, i.e. for an arbitrary locally finite real valued charge in Ω.

Remark 5.3 The formulation and the proof of Theorem 5.1 do not change if we assume that Ω is an open subset of an arbitrary Riemannian manifold.

Theorem 5.1 immediately gives the following criterion.

Corollary 5.2 *The trace inequality*

$$\int_\Omega |u|^2\, \mathbb{V}(dx) \leq C \int_\Omega |\nabla u|^2\, dx \tag{16}$$

holds for every $u \in C_0^\infty(\Omega)$ if and only if

$$\sup_{F \subset \Omega} \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} < \infty.$$

The bounds 1/4 and 1 in (14) and (15) are sharp. The gap between these sufficient and necessary conditions is the same as in Hille's non-oscillation criteria for the operator

$$-u'' - \mathbb{V}\, u, \qquad \mathbb{V} \geq 0,$$

on the positive semiaxis $\mathbb{R}^1_+$:

$$x\, \mathbb{V}((x,\infty)) \leq 1/4 \qquad \text{and} \qquad x\, \mathbb{V}((x,\infty)) \leq 1 \tag{17}$$

for all $x \geq 0$ [Hil]. By the way, conditions (17) are particular cases of (14) and (15) with $n = 1$ and $\Omega = \mathbb{R}^1_+$. $\square$

Combining Theorem 5.1 with isocapacitary inequalities (2)–(4), we arrive at sufficient conditions for (13) whose formulations involve no capacity. For example, in the two-dimensional case, (13) is guaranteed by the inequality

$$\mathbb{V}(F) \leq \frac{4\pi}{\log \dfrac{\mathrm{mes}_2\, \Omega}{\mathrm{mes}_2\, F}}.$$

The sharpness of this condition can be easily checked by analyzing the well known Hardy-type inequality

$$\int_\Omega \frac{|u(x)|^2}{|x|^2(\log|x|)^2}\, dx \leq 4 \int_\Omega |\nabla\, u(x)|^2\, dx,$$

where $u \in C_0^\infty(\Omega)$ and Ω is the unit disc. $\square$

The sufficiency of (14) for the inequality (13) can be directly obtained from the following more precise result.

Theorem 5.3 [Maz8] *Let $n \geq 1$ and let ν be a non-decreasing function on $(0, \infty)$ such that*

$$\mathbb{V}(F) \leq \nu(\mathrm{cap}_\Omega F)$$

for all compact subsets F of Ω. If

$$\int_0^\infty |v(\tau)|^2\, |d\nu(\tau^{-1})| \leq \int_0^\infty |v'(\tau)|^2 d\tau$$

for all absolutely continuous v with $v' \in L_2(0, \infty)$ and $v(0) = 0$, then (13) holds.

One example of the application of this assertion is the following improvement of the Hardy inequality which cannot be deduced from (14):

$$\int_{\mathbb{R}^n \setminus B_1} u^2 \Big(1 + \frac{1}{(n-2)^2(\log|x|)^2}\Big) \frac{dx}{|x|^2} \leq \frac{4}{(n-2)^2} \int_{\mathbb{R}^n \setminus B_1} |\nabla u|^2\, dx,$$

where $u \in C_0^\infty(\mathbb{R}^n \setminus \overline{B}_1)$ and $n > 2$. $\square$

Here is a dual assertion to Theorem 5.3 which is stated in terms of the Green function G of Ω and does not depend on the notion of capacity.

Theorem 5.4 *Let $\mathbb{V}_F$ be the restriction of the measure $\mathbb{V}$ to a compact set $F \subset \Omega$. Inequality (13) holds for every $u \in C_0^\infty(\Omega)$ provided*

$$\int_\Omega \int_\Omega G(x, y)\, \mathbb{V}_F(dx)\, \mathbb{V}_F(dy) \leq \frac{1}{4} \mathbb{V}(F) \tag{18}$$

for all F. Conversely, inequality (13) implies

$$\int_\Omega \int_\Omega G(x, y)\, \mathbb{V}_F(dx)\, \mathbb{V}_F(dy) \leq \mathbb{V}(F). \tag{19}$$

Sketch of the proof. Let u be a nonnegative function in $C_0^\infty(\Omega)$ such that $u \geq 1$ on F. Then

$$\mathbb{V}(F) \leq \int_\Omega u(x)\, \mathbb{V}_F(dx) \leq \Big(\int_\Omega \int_\Omega G(x, y)\, \mathbb{V}_F(dx)\, \mathbb{V}_F(dy)\Big)^{1/2} \|\nabla\, u\|_{L_2(\Omega)}$$

which in combination with (18) gives (14). The reference to Theorem 5.3 gives the sufficiency of (18).

Let (13) hold. Then

$$\Big|\int_\Omega u\,\mathbb{V}_F(dx)\Big|^2 \le \mathbb{V}(F)\,\|\nabla u\|^2_{L_2(\Omega)}.$$

Omitting a standard approximation argument, we put

$$u(x) = \int_\Omega G(x,y)\,\mathbb{V}_F(dy)$$

and the necessity of (19) results. $\square$

The next assertion follows directly from Theorem 7.1.

Corollary 5.5 *The trace inequality (16) holds if and only if there exists a constant $C > 0$ such that*

$$\int_F\int_F G(x,y)\,\mathbb{V}_F(dx)\,\mathbb{V}_F(dy) \le C\,\mathbb{V}(F) \tag{20}$$

for all compact sets F in Ω.

Remark 5.4 Note that Theorem 7.1 and Corollary 5.5 include the case $n = 2$ when the existence of the Green function is equivalent to $\mathrm{cap}(\mathbb{R}^2\backslash\Omega) > 0$ (see [Lan]).

Remark 5.5 Obviously, the pointwise estimate

$$\int_\Omega G(x,y)\,\mathbb{V}(dx) \le 1/4 \tag{21}$$

implies (18) and hence it is sufficient for (13) to hold. $\square$

It is well-known that the operator $\tilde{S}$ obtained by the closure of the quadratic form $S[u,u]$ defined by (12) generates a contractive semigroup on $L_p(\Omega)$, $p \in (1,\infty)$ if and only if

$$\int_\Omega |u|^{p-2}\,u\,\tilde{S}\,u\,dx \ge 0 \tag{22}$$

for all $u \in C_0^\infty(\Omega)$ ([LPh], [MS], [RS2], Th. X.48). The following analytic conditions related to (22) can be deduced from Theorem 5.1.

Corollary 5.6 *Let $p \in (1,\infty)$ and $p' = p/(p-1)$. The operator $\tilde{S}$ generates a contractive semigroup on $L_p(\Omega)$ if*

$$\sup_{F\subset\Omega} \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} \le \frac{1}{pp'}$$

and only if

$$\sup_{F\subset\Omega} \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} \le \frac{4}{pp'}.$$

6 Trace inequality for $\Omega = \mathbb{R}^n$

Inequality

$$\int_{\mathbb{R}^n} |u|^2\, \mathbb{V}(dx) \le C \int_{\mathbb{R}^n} |\nabla\, u|^2\, dx \tag{23}$$

deserves to be discussed in more detail. First, (23) for $n = 2$ implies $\mathbb{V} = 0$. Let $n > 2$. Needless to say, by Theorem 5.1 the condition

$$\sup_F \frac{\mathbb{V}(F)}{\mathrm{cap} F} < \infty, \tag{24}$$

where the supremum is taken over all compact sets F in $\mathbb{R}^n$, is necessary and sufficient for (23). Restricting ourselves to arbitrary balls B in $\mathbb{R}^n$, we have by (24) the obvious necessary condition

$$\sup_B \frac{\mathbb{V}(B)}{(\mathrm{mes}_n B)^{1-2/n}} < \infty. \tag{25}$$

On the other hand, using the isocapacitary inequality (4), we obtain the sufficient condition

$$\sup_F \frac{\mathbb{V}(F)}{(\mathrm{mes}_n F)^{1-2/n}} < \infty, \tag{26}$$

where the supremum is taken over all compact sets F in $\mathbb{R}^n$. Moreover, the best value of C in (23) satisfies

$$C \le \frac{4 v_n^{-2/n}}{n(n-2)} \sup_F \frac{\mathbb{V}(F)}{(\mathrm{mes}_n F)^{1-2/n}}$$

and the constant factor in front of the supremum is sharp [Maz3].

Although (25) and (26) look similar, they are not equivalent in general. In other words, one cannot replace arbitrary sets F in (24) by balls. Paradoxically, the situation with the criterion (20) in the case $\Omega = \mathbb{R}^n$ is different. In fact, Kerman and Sawyer [KeS] showed that the trace inequality (23) holds if and only if for all balls B in $\mathbb{R}^n$

$$\int_B \int_B \frac{\mathbb{V}(dx)\, \mathbb{V}(dy)}{|x-y|^{n-2}} \le C\, \mathbb{V}(B). \tag{27}$$

Maz'ya and Verbitsky [MV1] gave another necessary and sufficient condition for (23):

$$\sup_x \frac{I_1 (I_1 \mathbb{V})^2(x)}{I_1\, \mathbb{V}(x)} < \infty, \tag{28}$$

where I_s is the Riesz potential of order s, i.e.

$$I_s \mathbb{V}(x) := \int_{\mathbb{R}^n} \frac{\mathbb{V}(dy)}{|x-y|^{n-s}}.$$

The following complete characterization of (23) is due to Verbitsky [Ver]. For every dyadic cube P_0 in $\mathbb{R}^n$

$$\sup_{P_0} \frac{1}{V(P_0)} \sum \frac{\mathbb{V}(P)^2}{(\mathrm{mes}_n P)^{1-2/n}} < \infty, \tag{29}$$

where the sum is taken over all dyadic cubes P contained in P_0 and C does not depend on P_0.

Let us assume that $\mathbb{V}$ is absolutely continuous with respect to mes_n, i.e.

$$\mathbb{V}(F) = \int_F V(x)\,dx.$$

Fefferman and Phong [F] proved that (23) follows from

$$\sup_B \frac{\displaystyle\int_B V^t\,dx}{(\text{mes}_n B)^{1-2t/n}} < \infty \qquad \text{with some } t \in (1, n/2). \tag{30}$$

This can be readily deduced from Sawyer's inequality [Saw]

$$\int_{\mathbb{R}^n} (\mathcal{M}_t f)^2\,\nu(dx) \le C \sup_B \frac{\nu(B)}{(\text{mes}_n B)^{1-2t/n}} \int_{\mathbb{R}^n} f^2\,dx, \tag{31}$$

where ν is a measure, $f \ge 0$ and $\mathcal{M}_t$ is the fractional maximal operator defined by

$$\mathcal{M}_t f(x) = \sup_B \frac{\displaystyle\int_B f(y)\,dy}{(\text{mes}_n B)^{1-t/n}}.$$

In fact, for any $\delta > 0$

$$I_1 f(x) = (n-1)\int_0^\infty r^{-n} \int_{B_r(x)} f(y)\,dy\,dr \le (n-1)\big(\delta\,\mathcal{M}f(x) + (t-1)^{-1}\delta^{1-t}\mathcal{M}_t f(x)\big),$$

where $\mathcal{M}$ is the Hardy-Littlewood maximal operator. Minimizing the right-hand side in δ, we arrive at the inequality

$$I_1 f(x) \le \frac{(n-1)t}{t-1}\,(\mathcal{M}_t f(x))^{1/t}(\mathcal{M}\,f(x))^{1-1/t} \tag{32}$$

([Hed], see also [AH], Sect. 3.1). Now, (32) implies

$$\|I_1\,f\|_{L_2(V\,dx)} \le C\,\|\mathcal{M}_t f\|^{1/t}_{L_2(V^t dx)} \|\mathcal{M}\,f\|^{1-1/t}_{L_2(\mathbb{R}^n)}.$$

Therefore, by (31) and by the boundedness of $\mathcal{M}$ in $L_2(\mathbb{R}^n)$ we arrive at the inequality

$$\|I_1\,f\|_{L_2(V\,dx)} \le C\,\sup_B \left(\frac{\displaystyle\int_B V^t\,dx}{(\text{mes}_n B)^{1-2t/n}}\right)^{1/2t} \|f\|_{L_2(\mathbb{R}^n)}$$

which is equivalent to the Fefferman-Phong result. Their result was improved by Chang, Wilson and Wolff [ChWW] who showed that if φ is an increasing function $[0,\infty) \to [1,\infty)$ subject to

$$\int_1^\infty (\tau\,\varphi(\tau))^{-1} d\tau < \infty, \tag{33}$$

then the condition

$$\sup_B \frac{\displaystyle\int_B V(x)\,\varphi\big(V(x)(\text{diam}\,B)^2\big)\,dx}{(\text{mes}_n\,B)^{1-2/n}} < \infty \tag{34}$$

is sufficient for (23) to hold. The assumption (33) is sharp.

By Remark 5.5, the condition

$$\sup_x \int_{\mathbb{R}^n} \frac{\mathbb{V}(dy)}{|x-y|^{n-2}} < \infty, \tag{35}$$

is sufficient for (23). It is related to Kato's condition frequently used in the spectral theory of the Schrödinger operator (see Sect. 14 below for more information about Kato's condition). Note that (35) is rather far from being necessary since it excludes (23) with $\mathbb{V}(dx) = |x|^{-2}dx$, i.e. the classical Hardy inequality, unlike other conditions just mentioned.

We conclude this section with the observation that the multiplicative inequality

$$\int_{\mathbb{R}^n} u^2\, \mathbb{V}(dx) \le C \Big(\int_{\mathbb{R}^n} |\nabla u|^2 dx\Big)^{\tau} \Big(\int_{\mathbb{R}^n} u^2\, dx\Big)^{1-\tau}, \qquad 0 \le \tau < 1, \tag{36}$$

is equivalent to

$$\sup_B \frac{\mathbb{V}B}{(\mathrm{mes}_n B)^{1-2\tau/n}} < \infty \tag{37}$$

([Maz7], Theorem 1.4.7, see Sect. 15 below for further development).

7 Positive solutions of $(\Delta + \mathbb{V})w = 0$

Inequality (23) is intimately related to the problem of existence of positive solutions for the Schrödinger equation

$$-\Delta\, w = \mathbb{V}\, w \qquad \text{in } \mathbb{R}^n. \tag{38}$$

S. Agmon showed that the existence of $w \ge 0$ is equivalent to the positivity of the operator $-\Delta - \mathbb{V}$ for relatively nice $\mathbb{V}$ [Agm]. The following result due to Hansson, Maz'ya and Verbitsky [HMV] shows that the condition

$$I_1(I_1\mathbb{V})^2 \le C\, I_1\, \mathbb{V} \tag{39}$$

is equivalent (up to values of C) to the existence of $w > 0$.

Theorem 7.1 (i) *If $-\Delta\, w = \mathbb{V}\, w$ has a nonnegative (weak) solution w, then $I_1\mathbb{V} < \infty$ almost everywhere and there exists a constant $C_1 = C(n)$ such that*

$$I_1\big((I_1\mathbb{V})^2\big)(x) \le C_1\, I_1\, \mathbb{V}(x) \quad \text{a.e.} \tag{40}$$

(ii) *Conversely, there exists a constant $C_2 = C_2(n)$ such that if* (40) *holds with C_2 in place of C_1, then there exists a positive solution w to* (38) *which satisfies*

$$|\nabla\, \log\, w(x)| \le C\, I_1\, w(x)$$

and

$$w(x) \ge C\,(|x|+1)^{-c}$$

for some positive constants C and c.

In addition, if $I_2\mathbb{V}(x) < \infty$ a.e., then there is a solution w such that

$$e^{I_2\, \mathbb{V}(x)} \le w(x) \le e^{C\, I_2\, \mathbb{V}(x)}.$$

All the constants depend only on n.

8 Semiboundedness of the operator $-\Delta - \mathbb{V}$

We formulate some consequences of Theorem 5.1 concerning the topic in the title, i.e. the inequality

$$\int_\Omega |\nabla u|^2\, dx - \int_\Omega |u|^2\, \mathbb{V}(dx) \geq -C \int_\Omega |u|^2\, dx, \quad u \in C_0^\infty(\Omega).$$

Theorem 8.1 ([Maz3], see also [Maz7], Sect. 2.2)

(i) *If*

$$\limsup_{\delta\to 0} \Big\{ \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} : F \subset \Omega,\ \mathrm{diam}\, F \leq \delta \Big\} < \frac{1}{4}, \tag{41}$$

then the quadratic form $S[u,u]$ defined by (12) *is semi-bounded from below and closable in $L_2(\Omega)$.*

(ii) *If the form $S[u,u]$ is semi-bounded from below in $L_2(\Omega)$, then*

$$\limsup_{\delta\to 0} \Big\{ \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} : F \subset \Omega,\ \mathrm{diam}\, F \leq \delta \Big\} \leq 1. \tag{42}$$

Corollary 8.2 *The condition*

$$\limsup_{\delta\to 0} \Big\{ \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} : F \subset \Omega,\ \mathrm{diam}\, F \leq \delta \Big\} = 0 \tag{43}$$

is necessary and sufficient for the semiboundedness of the form

$$S_h[u,u] := h \int_\Omega |\nabla u|^2 dx - \int_\Omega |u|^2\, \mathbb{V}(dx) \tag{44}$$

in $L_2(\Omega)$ for all $h > 0$.

Corollary 8.3 *The inequality*

$$\int_\Omega |u|^2\, \mathbb{V}(dx) \leq C \int_\Omega (|\nabla u|^2 + |u|^2)\, dx, \tag{45}$$

where u is an arbitrary function in $C_0^\infty(\Omega)$ and C is a constant independent of u, holds if and only if there exists $\delta > 0$ such that

$$\sup\Big\{ \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} :\ F \subset \Omega,\ \mathrm{diam}\, F \leq \delta \Big\} < \infty.$$

9 Negative spectrum of $-h\Delta - \mathbb{V}$

Investigation of the negative spectrum of the Schrödinger operator with negative potential can be based upon the following two classical general results.

Lemma 9.1 [Fr] *Let $A[u,u]$ be a closed symmetric quadratic form in a Hilbert space H with domain $D[A]$ and let $\gamma(A)$ be its positive greatest lower bound. Further, let $B[u,u]$ be a real valued quadratic form, compact in $D[A]$. Then the form $A - B$ is semi-bounded below in H, closed in $D[A]$, and its spectrum is discrete to the left of $\gamma(A)$.*

Lemma 9.2 [Gl] *For the negative spectrum of a selfadjoint operator A to be infinite it is necessary and sufficient that there exists a linear manifold of infinite dimension on which* $(A\,u, u) < 0$.

Note also that by Birman's general theorem [Bir2], the discreteness of the negative spectrum of the operator

$$\tilde{S}_h = -h\Delta - \mathbb{V} \qquad \text{for all } h > 0$$

generated by the closure of the quadratic form $S_h[u, u]$ defined by (44) is equivalent to the compactness of the quadratic form

$$\int_\Omega |u|^2\, \mathbb{V}(dx) \tag{46}$$

with respect to the norm

$$\Big(\int_\Omega (|\nabla u|^2 + |u|^2)\, dx\Big)^{1/2}.$$

Analogously, the finiteness of the negative spectrum of the operator $\tilde{S}_h$ is equivalent to the compactness of the quadratic form (46) with respect to the norm $\|\nabla u\|_{L_2(\Omega)}$.

Moreover, by [Bir1] (see also [Bir2] and [Schw]) the number of negative eigenvalues of $\tilde{S}_h$ coincides with the number of eigenvalues λ_k, $\lambda_k < h^{-1}$, of the Dirichlet problem

$$-\Delta u - \lambda \mathbb{V}\, u = 0, \quad u \in \mathring{L}{}_2^1(\Omega).$$

The next theorem contains analytic conditions both necessary and sufficient for the Schrödinger operators $\tilde{S}_h$ to have discrete, infinite or finite negative spectra for all $h > 0$. These characterizations were obtained by the author from either sufficient or necessary conditions, analogous to (41), (42), for the operator $\tilde{S}$ independent of the parameter h to have a negative spectrum with the properties just listed ([Maz1], [Maz3], see also [Maz7], Sect. 2.2.)

Theorem 9.3 (i) *A necessary and sufficient condition for the discreteness of the negative spectrum of $\tilde{S}_h$ for all $h > 0$ is*

$$\sup_{F\subset\Omega\setminus B_\rho,\, \mathrm{diam} F\le 1} \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} \to 0 \quad \text{as } \rho \to \infty. \tag{47}$$

Here and elsewhere $B_\rho = \{x \in \mathbb{R}^n : |x| < \rho\}$.

(ii) *A necessary and sufficient condition for the discreteness of the negative spectrum of $\tilde{S}_h$ for all $h > 0$ is*

$$\sup_{F\subset\Omega\setminus B_\rho} \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} \to 0 \quad \text{as } \rho \to \infty. \tag{48}$$

(ii) *A necessary and sufficient condition for the negative spectrum of $\tilde{S}_h$ to be infinite for all $h > 0$ is*

$$\sup_{F\subset\Omega} \frac{\mathbb{V}(F)}{\mathrm{cap}_\Omega F} = \infty. \tag{49}$$

Needless to say, simpler sufficient conditions with $\mathrm{cap}_\Omega F$ replaced by a function of $\mathrm{mes}_n F$ follow directly from (47) - (49) and the isocapacitary inequalities (2) - (4).

10 Rellich-Kato theorem

By the basic Rellich-Kato theorem [Re1] - [Ka1], the self-adjointness of $-\Delta + V$ in $L_2(\mathbb{R}^n)$ is guaranteed by the inequality

$$\|V\,u\|_{L_2(\mathbb{R}^n)} \le a\,\|\Delta\,u\|_{L_2(\mathbb{R}^n)} + b\,\|u\|_{L_2(\mathbb{R}^n)}, \tag{50}$$

where $a < 1$ and u is an arbitrary function in $C_0^\infty(\mathbb{R}^n)$.

Let $n \le 3$. The Sobolev embedding $W_2^2(\mathbb{R}^n) \subset L_\infty(\mathbb{R}^n)$ and an appropriate choice of the test function in (50) show that (50) holds if and only if there is a sufficiently small constant $c(n)$ such that

$$\sup_{x\in\mathbb{R}^n} \int_{B_1(x)} |V(y)|^2\,dy \le c(n). \tag{51}$$

Here and elsewhere $B_r(x) = \{y \in \mathbb{R}^n : |y - x| < r\}$. This class of potentials is known as Stummel's class S_n which is defined also for higher dimensions by

$$\lim_{r\downarrow 0}\Big(\sup_x \int_{B_r(x)} |x-y|^{4-n}|V(y)|^2\,dy\Big) = 0 \qquad \text{for } n \ge 5,$$

$$\lim_{r\downarrow 0}\Big(\sup_x \int_{B_r(x)} \log(|x-y|^{-1})\,|V(y)|^2\,dy\Big) = 0 \qquad \text{for } n = 4,$$

[Stum]. Although the condition $V \in S_n$ is sufficient for (50) for every n, it does not seem quite natural for $n \ge 4$. As a matter of fact, it excludes the simple potential $V(x) = c|x|^{-2}$ obviously satisfying (50), if the factor c is small enough.

If $n \ge 5$, a characterization of (50) (modulo best constants) results directly from a necessary and sufficient condition for the inequality

$$\|V\,u\|_{L_2(\mathbb{R}^n)} \le C\,\|\Delta\,u\|_{L_2(\mathbb{R}^n)}, \qquad u \in C_0^\infty(\mathbb{R}^n),$$

found in [Maz4]. We claim that the Rellich-Kato condition (50) holds in the case $n \ge 4$ if and only if there is a sufficiently small $c(n)$ subject to

$$\sup_{\mathrm{diam} F \le 1} \frac{\displaystyle\int_F |V(y)|^2\,dy}{\mathrm{cap}_2 F} \le c(n) \tag{52}$$

(the values of $c(n)$ in the sufficiency and necessity parts are different similarly to the criteria in Sect. 4). Here and elsewhere cap_m is the polyharmonic capacity of a compact set F defined in the case $2m < n$ by

$$\mathrm{cap}_m F = \inf\Big\{\int_{\mathbb{R}^n} |\nabla_m\,u|^2\,dx : \ u \in C_0^\infty(\mathbb{R}^n),\, u \ge 1 \,\mathrm{on}\, F\Big\},$$

where $\nabla_m = \{\partial^m/\partial x_1^{\alpha_1}\dots\partial x_n^{\alpha_n}\}$. For $2m = n$ one should add $\|u\|^2_{L_2(\mathbb{R}^n)}$ to the last integral.

The condition

$$\sup_{\mathrm{diam} F \le \delta} \frac{\displaystyle\int_F |V(y)|^2\,dy}{\mathrm{cap}_2 F} \to 0 \quad \text{as } \delta \to 0 \tag{53}$$

is necessary and sufficient for (50) to hold with an arbitrary a and $b = b(a)$.

An obvious necessary condition for (50) is

$$\begin{cases} \sup\limits_{r\le 1, x\in\mathbb{R}^n} r^{4-n} \displaystyle\int_{B_r(x)} |V(y)|^2\, dy \le c(n) & \text{for } n\ge 5 \\ \sup\limits_{r\le 1, x\in\mathbb{R}^n} \big(\log \dfrac{2}{r}\big)^{-1} \displaystyle\int_{B_r(x)} |V(y)|^2\, dy \le c(n) & \text{for } n=4 \end{cases} \tag{54}$$

where $c(n)$ is sufficiently small. Standard lower estimates of cap_2 by mes_n combined with the criterion (52) give the sufficient condition

$$\begin{cases} \sup\limits_{\mathrm{diam} F\le 1} (\mathrm{mes}_n F)^{(4-n)/n} \displaystyle\int_F |V(y)|^2\, dy \le c(n) & \text{for } n\ge 5 \\ \sup\limits_{\mathrm{diam} F\le 1} \big(\log \dfrac{v_n}{\mathrm{mes}_n F}\big)^{-1} \displaystyle\int_F |V(y)|^2\, dy \le c(n) & \text{for } n=4. \end{cases} \tag{55}$$

Though sharp and looking similar, (54) and (55) are not equivalent. We omit a discussion of other sufficient and both necessary and sufficient conditions for (52) to hold parallel to that in Sect. 5 (analogs of the Fefferman & Phong, Kerman & Sawyer, Maz'ya & Verbitsky, and Verbitsky conditions mentioned in Sect. 5).

Finally, we observe that the inequality

$$\|V\,u\|_{L_2(\mathbb{R}^n)} \le C\, \|\Delta\, u\|^{\tau}_{L_2(\mathbb{R}^n)} \|u\|^{1-\tau}_{L_2(\mathbb{R}^n)}$$

holds for a certain $\tau\in(0,1)$ and every $u\in C_0^\infty(\mathbb{R})$ if and only if for all $r\in(0,1)$

$$\sup_x \int_{B_r(x)} |V(y)|^2\, dy \le C\, r^{n-4\tau}$$

(see Theorem 1.4.7 in [Maz7]).

11 Sobolev regularity for solutions of $(-\Delta+V)u=f$

Let m be integer ≥ 2 and let $W_2^m(\mathbb{R}^n)$ denote the Sobolev space of functions $u\in L_2(\mathbb{R}^n)$ such that $\nabla_m u\in L_2(\mathbb{R}^n)$. Obviously, the operator

$$-\Delta+V : W_2^m(\mathbb{R}^n)\to W_2^{m-2}(\mathbb{R}^n)$$

is bounded if and only if V is a pointwise multiplier acting from $W_2^m(\mathbb{R}^n)$ into $W_2^{m-2}(\mathbb{R}^n)$. (We use the notation $V\in M(W_2^m(\mathbb{R}^n)\to W_2^{m-2}(\mathbb{R}^n))$. According to [MSha1], Ch. 1, necessary and sufficient conditions for $V\in M(W_2^m(\mathbb{R}^n)\to W_2^{m-2}(\mathbb{R}^n)$ have the form

$$\sup_{x\in\mathbb{R}^n} \int_{B_1(x)} (|\nabla_{m-2}V(y)|^2 + |V(y)|^2)\, dy < \infty \tag{56}$$

for $n<2m$ and

$$\sup_{\mathrm{diam} F\le 1} \frac{\displaystyle\int_F |\nabla_{m-2}V(y)|^2\, dy}{\mathrm{cap}_m F} + \sup_{x\in\mathbb{R}^n} \int_{B_1(x)} |V(y)|^2\, dy < \infty \tag{57}$$

for $n\ge 2m$.

Two-sided estimates for the essential norm of a multiplier: $W_2^m(\mathbb{R}^n)\to W_2^{m-2}(\mathbb{R}^n)$ found in [MSha1], Ch. 4, lead to the following regularity result.

Theorem 11.1 *Let $\varphi \in W_2^1(\mathbb{R}^n, loc)$ be a solution of*

$$(-\Delta + V)\varphi = f,$$

where $f \in W_2^{m-2}(\mathbb{R}^n, loc)$.

If $n < 2m$ and $V \in W_2^{m-2}(\mathbb{R}^n, loc)$ then $\varphi \in W_2^{2m}(\mathbb{R}^n, loc)$.

Let $n \geq 2m$. Suppose there exists a sufficiently small constant $c(n)$ such that for all sufficiently small $\delta > 0$

$$\sup_{\mathrm{diam}F \leq \delta} \frac{\int_F |\nabla_{m-2} V(y)|^2 \, dy}{\mathrm{cap}_m F} + \sup_x \frac{\int_{B_\delta(x)} |V(y)|^2 \, dy}{\delta^{n-2m}} \leq c(n). \tag{58}$$

Then $\varphi \in W_2^{2m}(\mathbb{R}^n, loc)$.

Equivalent forms of the conditions (57) and (58) of Kerman & Sawyer, Maz'ya & Verbitsky, and Verbitsky type, as well as various separately necessary or sufficient conditions involving no capacities, are available (compare with Sect. 5).

Similar higher regularity L_p-results can be obtained from estimates of the essential norms of multipliers: $W_p^m(\mathbb{R}^n) \to W_p^{m-2}(\mathbb{R}^n)$ obtained in [MSha1], Ch. 4.

12 Relative form boundedness and form compactness

Maz'ya and Verbitsky [MV2] gave necessary and sufficient conditions for the inequality

$$\left| \int_{\mathbb{R}^n} |u(x)|^2 \, V(x) \, dx \right| \leq C \int_{\mathbb{R}^n} |\nabla u(x)|^2 \, dx, \quad u \in C_0^\infty(\mathbb{R}^n) \tag{59}$$

to hold. Here the "indefinite weight" V may change sign, or even be a complex-valued distribution on $\mathbb{R}^n$, $n \geq 3$. (In the latter case, the left-hand side of (59) is understood as $| < Vu, u > |$, where $< V \cdot, \cdot >$ is the quadratic form associated with the corresponding multiplication operator V.) An analogous inequality for the Sobolev space $W_2^1(\mathbb{R}^n)$, $n \geq 1$ was also characterized in [MV2]:

$$\left| \int_{\mathbb{R}^n} |u(x)|^2 \, V(x) \, dx \right| \leq C \int_{\mathbb{R}^n} \left(|\nabla u(x)|^2 + |u(x)|^2 \right) dx, \quad u \in C_0^\infty(\mathbb{R}^n). \tag{60}$$

Such inequalities are used extensively in spectral and scattering theory of the Schrödinger operator $H_V = -\Delta + V$ and its higher-order analogs, especially in questions of self-adjointness, resolvent convergence, estimates for the number of bound states, Schrödinger semigroups, etc. (See [Bir2], [BS1], [BS2], [CZh], [Dav1], [Far], [F], [RS2], [Sch1], [Sim3], and the literature cited there.) In particular, (60) is equivalent to the fundamental concept of the relative boundedness of the potential energy operator V with respect to $-\Delta$ in the sense of quadratic forms. Its abstract version appears in the so-called KLMN Theorem, which is discussed in detail together with applications to quantum-mechanical Hamiltonian operators, in [RS2], Sec. X.2.

It follows from the polarization identity that (59) can be restated equivalently in terms of the corresponding sesquilinear form:

$$| < Vu, v > | \leq C \, ||\nabla u||_{L_2} \, ||\nabla v||_{L_2},$$

for all $u, v \in C_0^\infty(\mathbb{R}^n)$. In other words, it is equivalent to the boundedness of the operator H_V,

$$H_V : \mathring{L}_2^1(\mathbb{R}^n) \to L_2^{-1}(\mathbb{R}^n), \qquad n \geq 3. \tag{61}$$

Here the energy space $\mathring{L}_2^1(\mathbb{R}^n)$ is defined as the completion of $C_0^\infty(\mathbb{R}^n)$ with respect to the Dirichlet norm $||\nabla u||_{L_2}$, and $L_2^{-1}(\mathbb{R}^n)$ is the dual of $\mathring{L}_2^1(\mathbb{R}^n)$. Similarly, (60) means that H is a bounded operator which maps $W_2^1(\mathbb{R}^n)$ to $W_2^{-1}(\mathbb{R}^n)$, $n \geq 1$.

Previously, the case of *nonnegative* V in (59) and (60) has been studied in a comprehensive way (see Sect. 5). For general V, only sufficient conditions have been known.

It is worthwhile to observe that the usual "naïve" approach is to decompose V into its positive and negative parts: $V = V_+ - V_-$, and to apply the just mentioned results to both V_+ and V_-. However, this procedure drastically diminishes the class of admissible weights V by ignoring a possible cancellation between V_+ and V_-. This cancellation phenomenon is evident for strongly oscillating weights considered below. Examples of this type are known mostly in relation to quantum mechanics problems [ASi], [CoG], [NS], [Stu].

The following result obtained in [MV2] reflects a general principle which has much wider range of applications.

Theorem 12.1 *Let V be a complex-valued distribution on $\mathbb{R}^n$, $n \geq 3$. Then* (59) *holds if and only if V is the divergence of a vector-field $\vec{\Gamma} : \mathbb{R}^n \to \mathbb{C}^n$ such that*

$$\int_{\mathbb{R}^n} |u(x)|^2 \, |\vec{\Gamma}(x)|^2 \, dx \leq \text{const} \int_{\mathbb{R}^n} |\nabla u(x)|^2 \, dx, \tag{62}$$

where the constant is independent of $u \in C_0^\infty(\mathbb{R}^n)$. The vector-field $\vec{\Gamma} \in \mathbf{L}_2(\mathbb{R}^n, loc)$ can be chosen as $\vec{\Gamma} = \nabla \Delta^{-1} V$.

Equivalently, the Schrödinger operator H_V acting from $\mathring{L}_2^1(\mathbb{R}^n)$ to $L_2^{-1}(\mathbb{R}^n)$ is bounded if and only if (62) *holds. Furthermore, the corresponding multiplication operator $V : \mathring{L}_2^1(\mathbb{R}^n) \to L_2^{-1}(\mathbb{R}^n)$ is compact if and only if the embedding*

$$\mathring{L}_2^1(\mathbb{R}^n) \subset L_2(\mathbb{R}^n, |\vec{\Gamma}|^2 \, dx)$$

is compact.

Once V is written as $V = \operatorname{div} \vec{\Gamma}$, the implication (62)→(59) becomes trivial. In fact, it follows using integration by parts and the Schwarz inequality. This idea has been known for a long time in mathematical physics (see, e.g., [CoG]) and theory of multipliers in Sobolev spaces [MSha1]. On the other hand, the proof of the converse statement (59)→(62) where $\vec{\Gamma} = \nabla \Delta^{-1} V$ is rather delicate.

Theorem 12.1 makes it possible to reduce the problems of boundedness and compactness for general "indefinite" V to the case of nonnegative weights $|\vec{\Gamma}|^2$, which is by now well understood. In particular, combining Theorem 12.1 and the criteria in Sect. 5 for $|\vec{\Gamma}|^2$ one arrives at analytic necessary and sufficient conditions for (59) to hold.

As a corollary, one obtains a necessary condition for (59) in terms of Morrey spaces of negative order.

Corollary 12.2 *If* (59) *holds, then, for every ball $B_r(x_0)$ of radius r,*

$$\int_{B_r(x_0)} |\nabla \Delta^{-1} V(x)|^2 \, dx \leq C \, r^{n-2},$$

where the constant does not depend on $x_0 \in \mathbb{R}^n$ and $r > 0$.

Corollary 12.3 *In the statements of Theorem 12.1 and Corollary 12.2, one can put the scalar function $(-\Delta)^{-\frac{1}{2}}V$ in place of $\vec{\Gamma} = \nabla\Delta^{-1}V$. In particular,* (62) *is equivalent to the inequality:*

$$\int_{\mathbb{R}^n} |u(x)|^2 \, |(-\Delta)^{-\frac{1}{2}}V(x)|^2 \, dx \le C \int_{\mathbb{R}^n} |\nabla u(x)|^2 \, dx, \tag{63}$$

for all $u \in C_0^\infty(\mathbb{R}^n)$.

The proof of Corollary 12.3 uses the boundedness of standard singular integral operators in the space of functions $f \in L_{2,\mathrm{loc}}(\mathbb{R}^n)$ such that

$$\int_{\mathbb{R}^n} |u(x)|^2 \, |f(x)|^2 \, dx \le C \int_{\mathbb{R}^n} |\nabla u(x)|^2 \, dx,$$

for all $u \in C_0^\infty(\mathbb{R}^n)$; this fact was established earlier in [MV1].

Corollary 12.3 indicates that a decomposition into a positive and negative part, appropriate for (59), should involve expressions like $(-\Delta)^{-\frac{1}{2}}V$ rather than V itself. Another important consequence is that the class of weights V satisfying (59) is invariant under standard singular integral and maximal operators.

Remark 12.1 Similar results are valid for inequality (60); one only has to replace the operator $(-\Delta)^{-1/2}$ with $(1-\Delta)^{-1/2}$, and the Wiener capacity $\operatorname{cap} F$ with the corresponding Bessel capacity (see [AH]). It suffices to restrict oneself, in the corresponding statements, to cubes or balls whose volumes are less than 1.

We now discuss some related results in terms of more conventional classes of admissible weights V. The following corollary, which is an immediate consequence of Theorem 12.1 and Corollary 12.3, gives a simpler sufficient condition for (59) with Lorentz-Sobolev spaces of negative order in its formulation.

Corollary 12.4 *Let $n \ge 3$, and let V be a distribution on $\mathbb{R}^n$ such that $(-\Delta)^{-\frac{1}{2}}V \in L_{n,\infty}(\mathbb{R}^n)$, where $L_{p,\infty}$ denotes the usual Lorentz (weak L_p) space. Then* (59) *holds.*

For the definition and basic properties of Lorentz spaces $L_{p,q}(\mathbb{R}^n)$ we refer to [SW]. Note that, in particular, $(-\Delta)^{-\frac{1}{2}}V \in L_{n,\infty}$ is equivalent to the estimate

$$\int_F |(-\Delta)^{-\frac{1}{2}}V(x)|^2 \, dx \le C \, (\mathrm{mes}_n F)^{1-2/n}. \tag{64}$$

The following corollary of Theorem 12.1 is applicable to distributions V, and encompasses a class of weights which is broader than the Fefferman−Phong class (30) even in the case where V is a nonnegative measurable function.

Corollary 12.5 *Let V be a distribution on $\mathbb{R}^n$ which satisfies, for some $t > 1$, the inequality*

$$\int_{B_r(x_0)} |(-\Delta)^{-\frac{1}{2}}V(x)|^{2t} \, dx \le C \, r^{n-2t}, \tag{65}$$

for every ball $B_r(x_0)$ in $\mathbb{R}^n$. Then (59) *holds.*

Note that by Corollary 12.2 the preceding inequality with $t = 1$ is necessary for (59) to hold.

Remark 12.2 A refinement of (65) in terms of the condition (34) established by Chang, Wilson, and Wolff [ChWW] is readily available by combining (34) with Theorem 12.1.

To clarify the multi-dimensional characterizations for "indefinite weights" V presented above, we state an elementary analog of Theorem 12.1 for the Sturm-Liouville operator $H_V = -\frac{d^2}{dx^2} + V$ on the half-line.

Theorem 12.6 *The inequality*

$$\left| \int_{\mathbb{R}_+} |u(x)|^2 \, V(x) \, dx \right| \le C \int_{\mathbb{R}_+} |u'(x)|^2 \, dx, \tag{66}$$

holds for all $u \in C_0^\infty(\mathbb{R}_+)$ *if and only if*

$$\sup_{a>0} \; a \int_a^\infty \left| \int_x^\infty V(t) \, dt \right|^2 dx < \infty, \tag{67}$$

where $\Gamma(x) = \displaystyle\int_x^\infty V(t) \, dt$ *is understood in terms of distributions.*

Equivalently, $H_V \, : \, \mathring{L}_2^1(\mathbb{R}_+) \to L_2^{-1}(\mathbb{R}_+)$ *is bounded if and only if* (67) *holds. Moreover, the corresponding multiplication operator* V *is compact if and only if*

$$a \int_a^\infty |\Gamma(x)|^2 \, dx = o\,(1), \qquad \text{where} \quad a \to 0^+ \quad \text{and} \quad a \to +\infty. \tag{68}$$

For nonnegative V, condition (67) is easily seen to be equivalent to the standard Hille condition [Hil]:

$$\sup_{a>0} \; a \int_a^\infty V(x) \, dx < \infty. \tag{69}$$

A similar statement is true for the compactness criterion (68).

13 Infinitesimal form boundedness

Maz'ya and Verbitsky [MV3] characterized the class of potentials $V \in \mathcal{D}'(\mathbb{R}^n)$ which are $-\Delta$-form bounded with relative bound zero, i.e., for every $\epsilon > 0$, there exists $C(\epsilon) > 0$ such that

$$|\langle Vu, \, u \rangle| \le \epsilon \, ||\nabla u||^2_{L_2(\mathbb{R}^n)} + C(\epsilon) \, ||u||^2_{L_2(\mathbb{R}^n)}, \quad \forall u \in C_0^\infty(\mathbb{R}^n). \tag{70}$$

In other words, they found necessary and sufficient conditions for the *infinitesimal form boundedness* of the potential energy operator V with respect to the kinetic energy operator $H_0 = -\Delta$ on $L_2(\mathbb{R}^n)$. Here V is an arbitrary real- or complex-valued potential (possibly a distribution). This notion appeared in relation to the KLMN theorem and has become an indispensable tool in mathematical quantum mechanics and PDE theory.

The preceding inequality ensures that, in case V is real-valued, a semi-bounded self-adjoint Schrödinger operator $H_V = H_0 + V$ can be defined on $L_2(\mathbb{R}^n)$ so that the domain of $Q[u, u]$ coincides with $W_2^1(\mathbb{R}^n)$. For complex-valued V, it follows that H_V is an m-sectorial operator on $L_2(\mathbb{R}^n)$ with $\text{Dom}(H_V) \subset W_2^1(\mathbb{R}^n)$ ([RS2], Sec. X.2; [EE], Sec. IV.4).

The characterization of (70) found in [MV3] uses only the functions $|\nabla(1-\Delta)^{-1} \, V|$ and $|(1-\Delta)^{-1} \, V|$, and is based on the representation:

$$V = \operatorname{div} \vec{\Gamma} + \gamma, \qquad \vec{\Gamma}(x) = -\nabla(1-\Delta)^{-1} \, V, \quad \gamma = (1-\Delta)^{-1} \, V. \tag{71}$$

In particular, it is shown that, necessarily, $\vec{\Gamma} \in L_2(\mathbb{R}^n, loc)^n, \quad \gamma \in L_1(\mathbb{R}^n, loc)$, and, when $n \geq 3$,

$$\lim_{\delta \to +0} \sup_{x_0 \in \mathbb{R}^n} \delta^{2-n} \int_{B_\delta(x_0)} \left(|\vec{\Gamma}(x)|^2 + |\gamma(x)| \right) dx = 0, \tag{72}$$

once (70) holds.

In the opposite direction, it follows from the results in [MV3] that (70) holds whenever

$$\lim_{\delta \to +0} \sup_{x_0 \in \mathbb{R}^n} \delta^{2r-n} \int_{B_\delta(x_0)} \left(|\vec{\Gamma}(x)|^2 + |\gamma(x)| \right)^r dx = 0, \tag{73}$$

where $r > 1$. Such admissible potentials form a natural analog of the Fefferman–Phong class (30) for the infinitesimal form boundedness problem where cancellations between the positive and negative parts of V come into play. It includes functions with highly oscillatory behavior as well as singular measures, and properly contains the class of potentials based on the original Fefferman–Phong condition where $|V|$ is used in (73) in place of $|\vec{\Gamma}|^2 + |\gamma|$. Moreover, one can expand this class further using the sharper condition (34) applied to $|\vec{\Gamma}|^2 + |\gamma|$.

A complete characterization of (70) obtained in [MV3] is given in the following theorem which provides for deducing explicit criteria of the infinitesimal form boundedness in terms of the *nonnegative* locally integrable functions $|\vec{\Gamma}|^2$ and $|\gamma|$.

Theorem 13.1 *Let $V \in \mathcal{D}'(\mathbb{R}^n)$, $n \geq 2$. The following statements are equivalent:*

(i) *V is infinitesimally form bounded with respect to $-\Delta$.*

(ii) *V has the form (71) where $\vec{\Gamma} = -\nabla(1-\Delta)^{-1} V$, $\gamma = (1-\Delta)^{-1} V$, and the measure $\mu \in M^+(\mathbb{R}^n)$ defined by*

$$d\mu = \left(|\vec{\Gamma}(x)|^2 + |\gamma(x)| \right) dx \tag{74}$$

has the property that, for every $\epsilon > 0$, there exists $C(\epsilon) > 0$ such that

$$\int_{\mathbb{R}^n} |u(x)|^2 \, d\mu \leq \epsilon \, ||\nabla u||^2_{L_2(\mathbb{R}^n)} + C(\epsilon) \, ||\nabla u||^2_{L_2(\mathbb{R}^n)}, \quad \forall u \in C_0^\infty(\mathbb{R}^n). \tag{75}$$

(iii) *For μ defined by (74),*

$$\lim_{\delta \to +0} \sup_{P_0 : \, \mathrm{diam}\, P_0 \leq \delta} \frac{1}{\mu(P_0)} \sum_{P \subseteq P_0} \frac{\mu(P)^2}{(\mathrm{mes}_n \, P)^{1-2/n}} = 0, \tag{76}$$

where P, P_0 are dyadic cubes in $\mathbb{R}^n$, i.e., sets of the form $2^i(k + [0,\,1)^n)$, where $i \in \mathbb{Z}$, $k \in \mathbb{Z}^n$.

(iv) *For μ defined by (74),*

$$\lim_{\delta \to +0} \sup_{F : \, \mathrm{diam}\, F \leq \delta} \frac{\mu(F)}{\mathrm{cap}\, F} = 0, \tag{77}$$

where F denotes a compact set of positive capacity in $\mathbb{R}^n$.

(v) *For μ defined by (74),*

$$\lim_{\delta \to +0} \sup_{x_0 \in \mathbb{R}^n} \frac{\left\| \mu_{B_\delta(x_0)} \right\|^2_{W_2^{-1}(\mathbb{R}^n)}}{\mu(B_\delta(x_0))} = 0, \tag{78}$$

where $\mu_{B_\delta(x_0)}$ is the restriction of μ to the ball $B_\delta(x_0)$.

(vi) *For μ defined by* (74),

$$\lim_{\delta\to+0}\ \sup_{x,\, x_0\in\mathbb{R}^n} \frac{G_1 * \left(G_1 * \mu_{B_\delta(x_0)}\right)^2(x)}{G_1 * \mu_{B_\delta(x_0)}(x)} = 0, \tag{79}$$

where $G_1 * \mu = (1-\Delta)^{-\frac{1}{2}}\mu$ is the Bessel potential of order 1.

In the one-dimensional case, the infinitesimal form boundedness of the Sturm-Liouville operator $H_V = -d^2/dx^2 + V$ on $L_2(\mathbb{R}^1)$ is actually a consequence of the form boundedness.

Theorem 13.2 *Let $V \in \mathcal{D}'(\mathbb{R}^1)$. Then the following statements are equivalent.*

(i) *V is infinitesimally form bounded with respect to $-d^2/dx^2$.*

(ii) *V is form bounded with respect to $-d^2/dx^2$, i.e.,*

$$|\langle V\, u,\, u\rangle| \le C\, ||u||^2_{W_2^1(\mathbb{R}^1)}, \quad \forall u \in C_0^\infty(\mathbb{R}^1).$$

(iii) *V can be represented in the form $V = d\Gamma/dx + \gamma$, where*

$$\sup_{x\in\mathbb{R}^1} \int_x^{x+1} \left(|\Gamma(x)|^2 + |\gamma(x)|\right)\, dx < +\infty. \tag{80}$$

(iv) *Condition* (80) *holds where*

$$\Gamma(x) = \int_{\mathbb{R}^1} \mathrm{sign}\,(x-t)\, e^{-|x-t|}\, V(t)\, dt, \qquad \gamma(x) = \int_{\mathbb{R}^1} e^{-|x-t|}\, V(t)\, dt$$

are understood in the distributional sense.

(v) *V belongs to the space $W_2^{-1}(\mathbb{R}^1, unif)$, with the norm*

$$\sup_{x\in\mathbb{R}^1} \|\eta(x-\cdot)\, V\|_{W_2^{-1}(\mathbb{R}^1)}, \qquad \text{where } \eta \in C_0^\infty(\mathbb{R}^1),\ \eta(0)=1.$$

The statement (iii)⇒(i) in Theorem 13.2 can be found in [Sch1], Theorem 11.2.1, whereas (ii)⇒(iv) follows from results in [MV2], Theorem 4.2 and [MV3], Theorem 2.5. The equivalence of (ii) and (v) is proved in [MSha2], Corollary 9. □

14 Kato's condition K_n

Among well-known sufficient conditions for (70) which ignore possible cancellations, we mention: $Q \in L^{\frac{n}{2}}(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$ $(n \ge 3)$ and $Q \in L^r(\mathbb{R}^2) + L^\infty(\mathbb{R}^2)$, $r > 1$ $(n = 2)$ (see [BrK]), as well as Kato's condition K_n introduced in [Ka2]:

$$\lim_{\delta\to+0}\ \sup_{x_0\in\mathbb{R}^n} \int_{B_\delta(x_0)} \frac{|Q(x)|}{|x-x_0|^{n-2}}\, dx = 0, \qquad n \ge 3, \tag{81}$$

$$\lim_{\delta\to+0}\ \sup_{x_0\in\mathbb{R}^n} \int_{B_\delta(x_0)} \log\frac{1}{|x-x_0|}\, |Q(x)|\, dx = 0, \qquad n = 2. \tag{82}$$

Kato's class proved to be especially important in studies of Schrödinger semi-groups, Dirichlet forms, and Harnack inequalities [Agm], [ASi], [Sim3]. Theorem 13.1 yields that (70) actually holds for a substantially broader class of potentials for which $|\vec{\Gamma}|^2 + |\gamma| \in K_n$. We emphasize that no *a priori* assumptions were imposed on $C(\epsilon)$ in this theorem.

An observation of Aizenman and Simon states that, under the hypothesis

$$C(\epsilon) \le a\, e^{b\, \epsilon^{-p}} \quad \text{for some } a, b > 0 \text{ and } 0 < p < 1,$$

all potentials V which obey (70) with $|V|$ in place of V are contained in Kato's class. This was first proved in [ASi] using the Feynman–Kac formalism. In [MV3], a sharp result of this kind is obtained with a simple analytic proof. It is shown that if (70) holds with $|V|$ in place of $V \in L^1_{\rm loc}(\mathbb{R}^n)$, then for any $C(\epsilon) > 0$,

$$\sup_{x_0 \in \mathbb{R}^n} \int_{B_\delta(x_0)} \frac{|V(x)|}{|x - x_0|^{n-2}}\, dx \le c \int_{\delta^{-2}}^{+\infty} \frac{\hat{C}(s)}{s^2}\, ds, \qquad n \ge 3, \tag{83}$$

$$\sup_{x_0 \in \mathbb{R}^2} \int_{B_\delta(x_0)} \log \frac{1}{|x - x_0|}\, |V(x)|\, dx \le c \int_{\delta^{-2}}^{+\infty} \frac{\hat{C}(s)}{s^2 \log s}\, ds, \qquad n = 2, \tag{84}$$

where c is a constant which depends only on n, and δ is sufficiently small. Here $\hat{C}(s) = \inf_{\epsilon > 0} \{C(\epsilon) + s\, \epsilon\}$ is the Legendre transform of $-C(\epsilon)$. In particular, it follows that the condition $C(\epsilon) \le a\, e^{b\, \epsilon^{-p}}$ for *any* $p > 0$ is enough to ensure that $V \in K_2$ in the more subtle two-dimensional case.

15 Trudinger's subordination for the Schrödinger operator

In [MV3] inequality (70) is studied also under the assumption that $C(\epsilon)$ has power growth, i.e., there exists $\epsilon_0 > 0$ such that

$$|\langle V u,\, u\rangle| \le \epsilon\, ||\nabla u||^2_{L_2(\mathbb{R}^n)} + c\, \epsilon^{-\beta}\, ||u||^2_{L_2(\mathbb{R}^n)}, \quad \forall u \in C_0^\infty(\mathbb{R}^n), \tag{85}$$

for every $\epsilon \in (0, \epsilon_0)$, where $\beta > 0$. Such inequalities appear in studies of elliptic PDE with measurable coefficients [Tru], and have been used extensively in spectral theory of the Schrödinger operator [ASi], [Ka2], [RS2], [RSS], [Sch1], [Dav1], [Dav2], [LPS], [Sim3].

As it turns out, it is still possible to characterize (85) using only $|\vec{\Gamma}|$ and $|\gamma|$ defined by (71), provided $\beta > 1$. It is shown in [MV3] that in this case (85) holds if and only if both of the following conditions hold:

$$\sup_{\substack{x_0 \in \mathbb{R}^n \\ 0 < \delta < \delta_0}} \delta^{2\frac{\beta-1}{\beta+1} - n} \int_{B_\delta(x_0)} |\vec{\Gamma}(x)|^2\, dx < +\infty, \tag{86}$$

$$\sup_{\substack{x_0 \in \mathbb{R}^n \\ 0 < \delta < \delta_0}} \delta^{\frac{2\beta}{\beta+1} - n} \int_{B_\delta(x_0)} |\gamma(x)|\, dx < +\infty, \tag{87}$$

for some $\delta_0 > 0$. However, in the case $\beta \le 1$ this is no longer true. For $\beta = 1$, (86) has to be replaced with the condition that $\vec{\Gamma}$ is in the local BMO space, or respectively is Hölder-continuous of order $(1 - \beta)/(1 + \beta)$ if $0 < \beta < 1$.

In the homogeneous case $\epsilon_0 = +\infty$, (85) is equivalent to the *multiplicative inequality* (36) where $\tau = \beta/(1 + \beta) \in (0,\, 1)$. In spectral theory, (36) is referred to as the form τ-subordination property (see, e.g., [Agr], [Gr1], [Gr2], [MM1], [RSS], Sec. 20.4).

For *nonnegative* potentials V, where V coincides with a locally finite measure μ on $\mathbb{R}^n$, inequality (36) is equivalent to (37) [Maz7], Sect. 1.4.7. For general V, the following result is obtained in [MV3]. If $\tau > 1/2$, then (36) holds if and only if $\nabla\Delta^{-1}V$ lies in the Morrey space $\mathcal{L}^{2,\lambda}(\mathbb{R}^n)$, where $\lambda = n+2-4\tau$. The Morrey space $\mathcal{L}^{r,\lambda}(\mathbb{R}^n)$ $(r>0, \lambda>0)$ consists of $f \in L^r(\mathbb{R}^n, loc)$ such that

$$\sup_{x_0\in\mathbb{R}^n,\,\delta>0} \frac{1}{|B_\delta(x_0)|^{\lambda/n}} \int_{B_\delta(x_0)} |f(x)|^r\,dx < +\infty.$$

We refer to [Pe] for the overview of Morrey spaces. For $\tau = 1/2$, (36) holds if and only if $\nabla\Delta^{-1}V \in \mathrm{BMO}(\mathbb{R}^n)$, and for $0<\tau<1/2$, whenever $\nabla\Delta^{-1}V$ is in the Hölder class $C^{1-2\tau}(\mathbb{R}^n)$. These different characterizations are equivalent to (37) if V is a nonnegative measure.

16 Discreteness of the spectrum of $-\Delta+\mathbb{V}$ with nonnegative potential

Friedrichs proved in 1934 [Fr] that to the left of the point $\lim\inf_{|x|\to\infty} V(x)$, the spectrum of the Schrödinger operator $H_V = -\Delta + V$ in $L_2(\mathbb{R}^n)$ with a locally integrable potential V is discrete, and hence all spectrum is discrete provided $V(x) \to +\infty$ as $|x| \to \infty$. By Rellich's criterion [Re2], the spectrum of H_V is purely discrete if and only if the ball $(H_V u, u) \le 1$ is a compact subset of $L_2(\mathbb{R}^n)$. This and the discreteness of spectrum easily imply that for every $d > 0$

$$\int_{Q_d} V(x)dx \to +\infty \quad \text{as} \quad Q_d \to \infty, \tag{88}$$

where Q_d is a closed cube with the edge length d and with the edges parallel to coordinate axes, $Q_d \to \infty$ means that the cube Q_d goes to infinity (with fixed d). In 1953 A.M.Molchanov [Mol] proved that this condition is in fact necessary and sufficient in case $n = 1$ but not sufficient for $n \ge 2$. He also discovered a modification of (88) which is equivalent to the discreteness of spectrum in the case $n \ge 2$:

$$\inf_F \int_{Q_d\setminus F} V(x)dx \to +\infty \quad \text{as} \quad Q_d \to \infty, \tag{89}$$

where infimum is taken over all compact subsets F of Q_d which are called *negligible*. The negligibility of F in the sense of Molchanov means that $\mathrm{cap}F \le \gamma\,\mathrm{cap}(Q_d)$, where cap is the Wiener capacity and $\gamma > 0$ is a sufficiently small constant. More precisely, Molchanov proved that one can take $\gamma = c_n$ where $\gamma = c_n = (4n)^{-4n}(\mathrm{cap}(Q_1))^{-1}$ for $n \ge 3$.

As early as in 1953, I.M.Gelfand raised the question about the best possible constant c_n (personal communication). We describe results from [MShu1], where a complete answer to this question is given.

Let $\mathbb{V}$ be a positive Radon measure in an open set $\Omega \subset \mathbb{R}^n$, absolutely continuous with respect to the Wiener capacity. We will consider the Schrödinger operator $H_{\mathbb{V}}$ which is formally given by the expression $-\Delta + \mathbb{V}$. It is defined in $L_2(\Omega)$ by the closure of the quadratic form $Q[u,u]$ with the domain $C_0^\infty(\Omega)$.

Instead of the cubes Q_d, a more general family of test bodies will be used. Let us start with a standard open set $\mathcal{G} \subset \mathbb{R}^n$. We assume that $\mathcal{G}$ satisfies the following conditions:

(a) $\mathcal{G}$ is bounded and star-shaped with respect to the ball B_ρ;

(b) $\mathrm{diam}(\mathcal{G}) = 1$.

For any positive $d > 0$ denote by $\mathcal{G}_d(0)$ the body $\{x : \ d^{-1}x \in \mathcal{G}\}$ which is homothetic to $\mathcal{G}$ with coefficient d and with the center of homothety at 0. We will denote by $\mathcal{G}_d$ a body which is obtained from $\mathcal{G}_d(0)$ by a parallel translation: $\mathcal{G}_d(y) = y + \mathcal{G}_d(0)$ where y is an arbitrary vector in $\mathbb{R}^n$.

The notation $\mathcal{G}_d \to \infty$ means that the distance from $\mathcal{G}_d$ to 0 goes to infinity.

Definition. Let $\gamma \in (0,1)$. The *negligibility class* $\mathcal{N}_\gamma(\mathcal{G}_d;\Omega)$ consists of all compact sets $F \subset \overline{\mathcal{G}}_d$ satisfying the following conditions:

$$\bar{\mathcal{G}}_d \setminus \Omega \subset F \subset \bar{\mathcal{G}}_d \ , \tag{90}$$

and

$$\operatorname{cap} F \leq \gamma \operatorname{cap} \bar{G}_d. \tag{91}$$

Now we formulate the main result of the work in [MShu1] about the discreteness of spectrum.

Theorem 16.1 (i) (Necessity) *Let the spectrum of $H_{\mathbb{V}}$ be discrete. Then for every function $\gamma : (0,+\infty) \to (0,1)$ and every $d > 0$*

$$\inf_{F \in \mathcal{N}_{\gamma(d)}(\mathcal{G}_d,\Omega)} \mathbb{V}(\bar{\mathcal{G}}_d \setminus F) \to +\infty \quad \text{as} \quad \mathcal{G}_d \to \infty. \tag{92}$$

(ii) (Sufficiency) *Let a function $d \to \gamma(d) \in (0,1)$ be defined for $d > 0$ in a neighborhood of 0, and satisfy*

$$\limsup_{d \downarrow 0} d^{-2}\,\gamma(d) = +\infty. \tag{93}$$

Assume that there exists $d_0 > 0$ such that(92) holds for every $d \in (0, d_0)$. Then the spectrum of $H_{\mathbb{V}}$ in $L_2(\Omega)$ is discrete.

Let us make some comments about this theorem.

Remark 16.1 It suffices for the discreteness of spectrum of $H_{\mathbb{V}}$ that the condition (92) holds only for a sequence of d's, i.e. $d \in \{d_1, d_2, \ldots\}$, $d_k \to 0$ and $d_k^{-2}\gamma(d_k) \to +\infty$ as $k \to +\infty$.

Remark 16.2 The condition (92) in the sufficiency part can be replaced by a weaker requirement: there exist $c > 0$ and $d_0 > 0$ such that for every $d \in (0, d_0)$ there exists $R > 0$ such that

$$d^{-n} \inf_{F \in \mathcal{N}_{\gamma(d)}(\mathcal{G}_d,\Omega)} \mathbb{V}(\bar{\mathcal{G}}_d \setminus F) \geq c d^{-2}\gamma(d), \tag{94}$$

whenever $\bar{\mathcal{G}}_d \cap (\Omega \setminus B_R) \neq \emptyset$ (i.e. for distant bodies $\mathcal{G}_d$ having non-empty intersection with Ω). Moreover, it suffices that the condition (94) is satisfied for a sequence $d = d_k$ satisfying the condition formulated in Remark 16.1.

Note that unlike (92), the condition (94) does not require that the left-hand side goes to $+\infty$ as $\mathcal{G}_d \to \infty$. What is actually needed is that the left-hand side has a certain lower bound, depending on d for arbitrarily small $d > 0$ and distant test bodies $\mathcal{G}_d$. Nevertheless, the conditions (92) and (94) are equivalent because each is equivalent to the discreteness of spectrum.

Remark 16.3 If we take $\gamma = \mathit{const} \in (0,1)$, then Theorem 16.1 gives Molchanov's result, but with the constant $\gamma = c_n$ replaced by an arbitrary constant $\gamma \in (0,1)$. So Theorem 16.1 contains an answer to the above-mentioned Gelfand's question.

Remark 16.4 For any two functions $\gamma_1, \gamma_2 : (0, +\infty) \to (0, 1)$ satisfying the requirement (93), the conditions (92) are equivalent, and so are the conditions (94), because any of these conditions is equivalent to the discreteness of spectrum.

It follows that the conditions (92) for different constants $\gamma \in (0, 1)$ are equivalent. In the particular case, when the measure $\mathbb{V}$ is absolutely continuous with respect to the Lebesgue measure, we see that the conditions (89) with different constants $\gamma \in (0, 1)$ are equivalent.

Remark 16.5 The results above are new even for the operator $-\Delta$ in $L_2(\Omega)$ (for an arbitrary open set $\Omega \subset \mathbb{R}^n$ with the Dirichlet boundary conditions on $\partial\Omega$). In this case the discreteness of spectrum is completely determined by the geometry of Ω. More precisely, for the discreteness of spectrum of H_0 in $L_2(\Omega)$ it is necessary and sufficient that there exists $d_0 > 0$ such that for every $d \in (0, d_0)$

$$\liminf_{\mathcal{G}_d \to \infty} \operatorname{cap}(\bar{\mathcal{G}}_d \setminus \Omega) \geq \gamma(d) \operatorname{cap} \bar{\mathcal{G}}_d, \tag{95}$$

where $d \to \gamma(d) \in (0, 1)$ is a function, which is defined in a neighborhood of 0 and satisfies (93). The conditions (95) with different functions γ, satisfying the conditions above, are equivalent. This is a non-trivial property of capacity. It is necessary for the discreteness of spectrum that (95) holds for every function $\gamma : (0, +\infty) \to (0, 1)$ and every $d > 0$, but this condition may not be sufficient if γ does not satisfy (93) (see Theorem 16.2 below).

The following result demonstrates that the condition (93) is precise.

Theorem 16.2 *Assume that $\gamma(d) = O(d^2)$ as $d \to 0$. Then there exists an open set $\Omega \subset \mathbb{R}^n$ and $d_0 > 0$ such that for every $d \in (0, d_0)$ the condition (95) is satisfied but the spectrum of $-\Delta$ in $L_2(\Omega)$ with the Dirichlet boundary conditions is not discrete.*

17 Strict positivity of the spectrum of $-\Delta + \mathbb{V}$

We say that the operator $H_{\mathbb{V}}$, the same as in Sect. 11, is *strictly positive* if its spectrum does not contain 0. Equivalently, we can say that the spectrum is separated from 0. The strict positivity is equivalent to the existence of $\lambda > 0$ such that

$$Q[u, u] \geq \lambda \|u\|^2_{L_2(\Omega)}, \quad u \in C_0^\infty(\Omega). \tag{96}$$

The characterization of positivity of the spectrum in the next theorem with Molchanov's negligible sets in the formulation was found in [Maz5] (see also [Maz7], Sect. 12.5). The present stronger version is obtained by Maz'ya and Shubin in [MShu1].

Theorem 17.1 (i) (Necessity) *Let us assume that $H_{\mathbb{V}}$ is strictly positive, so that (96) is satisfied with a constant $\lambda > 0$. Let us take an arbitrary $\gamma \in (0, 1)$. Then there exist $d_0 > 0$ and $\varkappa > 0$ such that*

$$d^{-n} \inf_{F \in \mathcal{N}_\gamma(\mathcal{G}_d, \Omega)} \mathbb{V}(\bar{\mathcal{G}}_d \setminus F) \geq \varkappa \tag{97}$$

for every $d > d_0$ and every $\mathcal{G}_d$.

(ii) (Sufficiency) *Assume that there exist $d > 0$, $\varkappa > 0$ and $\gamma \in (0, 1)$, such that (97) is satisfied for every $\mathcal{G}_d$. Then the operator $H_{\mathbb{V}}$ is strictly positive.*

Instead of all bodies $\mathcal{G}_d$ it is sufficient to take only the ones from a finite multiplicity covering (or tiling) of $\mathbb{R}^n$.

Remark 17.1 Considering the Dirichlet Laplacian in $L_2(\Omega)$ we see from Theorem 17.1 that for any choice of a constant $\gamma \in (0,1)$ and a standard body $\mathcal{G}$, the strict positivity of $-\Delta$ is equivalent to the following condition

$$\exists\, d > 0, \text{ such that } \operatorname{cap}(\bar{\mathcal{G}}_d \cap (\mathbb{R}^n \backslash \Omega)) \geq \gamma \operatorname{cap}(\bar{\mathcal{G}}_d) \text{ for all } \mathcal{G}_d. \tag{98}$$

In particular, it follows that for two different γ's these conditions are equivalent. Noting that $\mathbb{R}^n \backslash \Omega$ can be an arbitrary closed subset in $\mathbb{R}^n$, we get a property of the Wiener capacity, which is obtained as a byproduct of our spectral theory arguments.

18 Two-sided estimates for the bottom of spectrum and essential spectrum

Let $\lambda = \lambda(\Omega, H_{\mathbb{V}})$ denote the greatest lower bound of the spectrum of the Schrödinger operator $H_{\mathbb{V}}$ handled in the two preceding sections. By $\mathcal{Q}_\Omega$ we denote the set of all cubes Q_d having a negligible intersection with the complement of Ω (in Molchanov's sense), i.e.

$$\mathcal{Q}_\Omega = \{Q_d : \operatorname{cap}(Q_d \setminus \Omega) \leq \gamma \operatorname{cap} Q_d\}, \tag{99}$$

where γ is sufficiently small.

For $\mathbb{V} = 0$ Maz'ya [Maz6] and for the general case Maz'ya and Otelbaev [MaO] (see also [Maz7], Ch. 12) obtained the two-sided estimate

$$c_1 D^{-2} \leq \lambda \leq c_2 D^{-2}, \tag{100}$$

with $D = D(\Omega, \mathbb{V})$ given by

$$D = \sup_{Q_d \in \mathcal{Q}_\Omega} \left\{ d : \; d^{n-2} \geq \inf_F \mathbb{V}(Q_d \backslash F) \right\}. \tag{101}$$

Here c_1 and c_2 are positive constants which depend only upon n and the infimum is taken over all sets F, satisfying

$$Q_d \setminus \Omega \subset F \subset Q_d \quad \text{and} \quad \operatorname{cap} F \leq \gamma \operatorname{cap} Q_d.$$

Clearly, the strict positivity of $H_{\mathbb{V}}$ is equivalent to the condition $D < \infty$.

In particular, if $\mathbb{V} = 0$, then D becomes the capacitary interior diameter of Ω: the maximal size d of cubes Q_d with the negligible intersection with $\mathbb{R}^n \setminus \Omega$ (i.e. cubes $Q_d \in \mathcal{Q}_\Omega$). The notion of the capacitary interior diameter was introduced in [Maz6]. Explicit estimates for c_1 and c_2 in the case $\mathbb{V} = 0$ are given in [MShu2], where also the smallness condition of γ is replaced with $\gamma \in (0,1)$.

The paper [MaO] (see also [Maz7], Ch. 12) also contains a two-sided estimate for the bottom of the essential spectrum of $H_{\mathbb{V}}$ in $L_2(\Omega)$. We will denote this bottom by $\Lambda = \Lambda(\Omega; H_{\mathbb{V}})$. The estimate has the form

$$c_1 D_\infty^{-2} \leq \Lambda \leq c_2 D_\infty^{-2}, \tag{102}$$

where

$$D_\infty = \lim_{R \to \infty} D(\Omega \setminus \bar{B}_R, \mathbb{V}, \gamma). \tag{103}$$

Note that the discreteness of spectrum of $H_{\mathbb{V}}$ is equivalent to the equality $\Lambda = +\infty$. Therefore, (102) implies that $D_\infty = 0$ is necessary and sufficient for the pure discreteness of the spectrum of $H_{\mathbb{V}}$.

In the recent work [Tay] M. Taylor found another criterion of discreteness of the spectrum of $H_{\mathbb{V}}$ stated in terms of the so-called scattering length of $\mathbb{V}$.

19 Structure of the essential spectrum of $H_{\mathbb{V}}$

We use the same notation as in Sections 16–18. The following result is due to Glazman [Gl].

Lemma 19.1 *If the spectrum of $H_{\mathbb{V}}$ is not purely discrete, the essential spectrum of $H_{\mathbb{V}}$ extends to infinity. Moreover, if 0 belongs to the essential spectrum of $H_{\mathbb{V}}$, then this spectrum coincides with $[0,\infty)$.*

Proof. Let Λ be the bottom of the essential spectrum. Then there exists a sequence of real-valued functions $\{\varphi_\nu\}_{\nu\geq 1}$ in $C_0^\infty(\Omega)$ subject to the conditions

$$\|\varphi_\nu\|_{L_2(\Omega)} = 1, \qquad \varphi_\nu \to 0 \quad \text{weakly in } L_2(\Omega), \tag{104}$$

$$\|(H_{\mathbb{V}} - \Lambda)\,\varphi_\nu\|_{L_2(\Omega)} \to 0. \tag{105}$$

We set

$$u_\nu = \varphi_\nu \exp\Big(i(\alpha-\Lambda)^{1/2}\sum_{k=1}^n x_k\Big),$$

where $\alpha > \Lambda$. We see that u_ν satisfies (104) and that

$$\|(H_{\mathbb{V}} - \alpha)\,u_\nu\|^2_{L_2(\Omega)} = \|(H_{\mathbb{V}} - \Lambda)\,\varphi_\nu\|^2_{L_2(\Omega)} + 4(\alpha-\Lambda)\|\sum_{k=1}^n \partial\varphi_\nu/\partial x_k\|^2_{L_2(\Omega)}.$$

Since the right-hand side does not exceed

$$\|(H_{\mathbb{V}} - \Lambda)\,\varphi_\nu\|^2_{L_2(\Omega)} + 4(\alpha-\Lambda)\,Q[\varphi_\nu,\varphi_\nu],$$

we have

$$\|(H_{\mathbb{V}} - \alpha)\,u_\nu\|^2_{L_2(\Omega)} \leq \|(H_{\mathbb{V}} - \Lambda)\,\varphi_\nu\|^2_{L_2(\Omega)}$$
$$+4n(\alpha-\Lambda)\,\|(H_{\mathbb{V}} - \Lambda)\,\varphi_\nu\|_{L_2(\Omega)} + 4n\Lambda(\alpha-\Lambda).$$

By (105)

$$\limsup_{\nu\to\infty} \|(H_{\mathbb{V}} - \alpha)\,u_\nu\|_{L_2(\Omega)} \leq \rho(\alpha),$$

where $\rho(\alpha) = 2(n\,\Lambda(\alpha-\Lambda))^{1/2}$. It follows that any segment $[\alpha-\rho(\alpha), \alpha+\rho(\alpha)]$ contains points of the essential spectrum. If, in particular, $\Lambda = 0$ then every positive α belongs to the essential spectrum. $\square$

In concert with this lemma the pairs $(\Omega,\mathbb{V})$ can be divided into three non-overlapping classes. The first class includes $(\Omega,\mathbb{V})$ such that the spectrum of $H_{\mathbb{V}}$ is discrete. The pair $(\Omega,\mathbb{V})$ belongs to the second class if the essential spectrum of $H_{\mathbb{V}}$ is unbounded and strictly positive. Finally, $(\Omega,\mathbb{V})$ is of the third class if the essential spectrum of $H_{\mathbb{V}}$ coincides with $[0,\infty)$.

By (101) and (102) the three classes can be described as follows:

(i) $(\Omega,\mathbb{V})$ belongs to the first class if and only if $D_\infty = 0$.

(ii) $(\Omega,\mathbb{V})$ belongs to the second class if and only if $D_\infty > 0$.

(iii) $(\Omega,\mathbb{V})$ belongs to the third class if and only if $D = \infty$ (or, equivalently, $D_\infty = \infty$).

By Theorem 16.1, the condition (i) is equivalent to (92) and (ii) holds if and only if (97) is valid. Finally, (iii) is equivalent to the failure of (95) by Theorem 17.1 and Lemma 19.1. In other words, (iii) holds if and only if

$$\liminf_{\mathcal{G}_d\to\infty}\ \inf_{F\in\mathcal{N}_{\gamma(d)}(\mathcal{G}_d,\Omega)} \mathbb{V}(\bar{\mathcal{G}}_d\setminus F) = 0$$

for every $d > 0$.

There are still open problems in the study of conditions insuring the absolute continuity of the spectrum. B. Simon conjectured in [Sim5] that the absolutely continuous spectrum of H_V with V subject to

$$\int_{\mathbb{R}^n} (V(x))^2 (1+|x|)^{1-n}\, dx < \infty$$

is the positive real axis. An interesting sufficient condition supporting this conjecture:

$$V = \operatorname{div} \vec{\Gamma} \quad \text{and} \quad |V(x)| + |\vec{\Gamma}(x)| \le c\,(1+|x|)^{-1/2-\varepsilon}, \;\; \varepsilon > 0,$$

has been obtained recently by Denisov in [Den].

20 Two measure boundedness and compactness criteria

The following lemma is a particular case of a more general result from [Maz4] (see also [Maz7], Sect. 2.3.7).

Lemma 20.1 *Let μ and ν be two nonnegative Radon measures in $\Omega \subset \mathbb{R}^n$, $n \ge 1$. The inequality*

$$\int_\Omega |u|^2\, d\mu \le C\Big(\int_\Omega |\nabla u|^2\, dx + \int_\Omega |u|^2\, d\nu\Big) \tag{106}$$

holds for all $u \in C_0^\infty(\Omega)$ if and only if there exists a constant $K > 0$ such that for all open bounded sets g and G subject to $\bar{g} \subset G$, $\bar{G} \subset \Omega$, the inequality

$$\mu(g) \le K(\operatorname{cap}_G \bar{g} + \nu(G)) \tag{107}$$

holds.

This criterion becomes more transparent in the one-dimensional case because the capacity admits an explicit representation.

Theorem 20.2 (see [Maz9]) *Let $n = 1$ and let σ_d denote the open interval $(x-d, x+d)$. Inequality*

$$\int_\Omega |u|^2\, d\mu \le C\Big(\int_\Omega |u'|^2\, dx + \int_\Omega |u|^2\, d\nu\Big) \tag{108}$$

holds for all $u \in C_0^\infty(\Omega)$ if and only if

$$\mu(\sigma_d(x)) \le const(\tau^{-1} + \nu(\sigma_{d+\tau}(x))), \tag{109}$$

where x, d, and τ are such that $\overline{\sigma_{d+\tau}(x)} \subset \Omega$, is valid without complementary assumptions about μ and ν. The sharp constant C in (108) is equivalent to

$$\sup_{x,d,\tau} \frac{\mu(\sigma_d(x))}{\tau^{-1} + \nu(\sigma_{d+\tau}(x))},$$

where x, d, and τ are the same as in (109).

We define the space $\mathring{W}_2^1(\nu)$ as the closure of $C_0^\infty(\Omega)$ with respect to the norm

$$\|f\|_{\mathring{W}_2^1(\nu)} = \Big(\int_\Omega |f'(x)|^2\,dx + \int_\Omega |f(x)|^2\,d\nu\Big)^{1/2}.$$

The condition (109) is a criterion of boundedness for the embedding operator $I : \mathring{W}_2^1(\nu) \to L_2(\mu)$.

The next theorem contains a two-sided estimate for the essential norm of I. We recall that the essential norm of a bounded linear operator A acting from X into Y, where X and Y are linear normed spaces, is defined by

$$\operatorname{ess}\|A\| = \inf_T \|A - T\|$$

with infimum taken over all compact operators $T : X \to Y$.

Theorem 20.3 [Maz9] *Let*

$$E(\mu,\nu) : \lim_{M\to\infty} \sup_{x,d,\tau} \frac{\mu(\sigma_d(x)\backslash[-M,M])}{\tau^{-1} + \nu(\sigma_{d+\tau}(x))}.$$

There exist positive constants c_1 and c_2 such that

$$c_1\,E(\mu,\nu)^{1/2} \le \operatorname{ess}\|I\| \le c_2\,E(\mu,\nu)^{1/2}. \tag{110}$$

In particular, the operator I is compact if and only if

$$\lim_{M\to\infty} \sup_{x,d,\tau} \frac{\mu(\sigma_d(x)\backslash[-M,M])}{\tau^{-1} + \nu(\sigma_{d+\tau}(x))} = 0,$$

where x, d, and τ are the same as in (109).

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