

DECAY OF EIGENFUNCTIONS OF ELLIPTIC PDE'S, I

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ABSTRACT. We study exponential decay of eigenfunctions of self-adjoint higher order elliptic operators on \mathbb{R}^d . We show that the possible (global) critical decay rates are determined algebraically. In addition we show absence of super-exponentially decaying eigenfunctions and a refined exponential upper bound.

CONTENTS

1. Introduction and results	1
1.1. Results	3
1.2. Principal example, $Q(\xi) - \lambda = G(\xi^2)$	5
1.3. Local critical decay rate	6
1.4. Notation and some calculus considerations	7
2. Ideas of proof of Theorems 1.2 and 1.3	8
3. Preliminaries	9
3.1. Calculus of pseudodifferential operators	9
3.2. Exponentially conjugated operator	11
3.3. Exponentially weighted Sobolev estimate	11
3.4. More elliptic estimates	12
4. A priori energy localization	14
4.1. Sobolev regularity bounds	14
4.2. Refined energy bounds	14
4.3. Other parameter-dependent bounds	17
5. Proof of Theorem 1.2 i)	18
6. Proof of Theorem 1.3	18
7. Proof of Theorem 1.2 ii)	20
8. Proof of Theorem 1.1	21
9. Proof of Theorems 1.4 and 1.5	23
9.1. Calculation of a commutator	23
9.2. Proof of Theorem 1.4	26
9.3. Symmetrized estimate	26
9.4. Proof of Theorem 1.5	28
References	30

1. INTRODUCTION AND RESULTS

Consider a real elliptic polynomial Q of degree q on \mathbb{R}^d . We consider the operator $H = Q(p) + V(x)$, $p = -i\nabla$, on $L^2 = L^2(\mathbb{R}^d)$ with V real-valued, bounded and measurable and with $\lim_{|x| \rightarrow \infty} V(x) = 0$. By the assumptions on Q the operator $Q(p)$ is self-adjoint on the standard Sobolev space of order q which consequently

Key words and phrases. eigenfunctions, exponential decay, microlocal analysis, combinatorics.

is the domain of H too. The goal of the paper is to study exponential decay of L^2 -eigenfunctions of H . It is the first in a series of two papers on the subject, the second one is [HS].

We will mostly assume there is a splitting of V , $V = V_1 + V_2$, into real-valued bounded functions, V_1 smooth and V_2 measurable, with additional assumptions depending on the result. With virtually no complication of proofs V_2 could be taken complex-valued.

For a given $\lambda \in \mathbb{R}$ the energy surface

$$S_\lambda = \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d \mid Q(\xi) = \lambda\}$$

is by definition regular if λ is not a critical value of Q , that is if

$$\nabla Q(\xi) \neq 0 \text{ on } S_\lambda. \tag{1.1}$$

We will need this condition in one of our results.

Suppose $(H - \lambda)\phi = 0$, $\phi \in L^2$. The *critical decay rate* is defined as

$$\sigma_c = \sup\{\sigma \geq 0 \mid e^{\sigma|x|}\phi \in L^2\}.$$

In this paper we shall study this notion of global decay rate for eigenfunctions, cf. previous works for the Laplacian [CT, FHH2O1, FHH2O2, FHH2O3] corresponding to the case $Q(\xi) = \xi^2$. We devote [HS] to the study of the so-called local critical decay rate, see Subsection 1.3 for a definition and an announcement of some results of the second paper of this series. In particular we give in the present paper necessary (phase-space) conditions for a positive number σ to be the critical decay rate (generalizing a result for the Laplacian), and we shall give a refined exponential upper bound (actually a new result for the Laplacian). This set of conditions defines a notion of *exceptional points* playing the same role as a certain set for the N -body problem related to the set of thresholds [FH, IS1]. However these conditions are very different from what could be expected from this analogous problem. More precisely the critical decay rate is not computable in terms of the critical values of Q which are the exceptional energies for the Mourre estimate [Mo] if we use the “natural” conjugate operator $A = x \cdot \nabla Q(p) + \nabla Q(p) \cdot x$. On the other hand, as we shall see, $\sigma_c > 0$ at non-critical values. A similar partial result, although in different settings, appears in [MP1, MP2].

To be a little more precise about the analogy of our problem with the N -body problem let us add a sufficiently decaying N -particle interaction potential to the N -body Hamiltonian (which produces a potential decaying in the whole space after the center of mass motion is removed). Then the possible decay rates are independent of this potential just as they are independent of our decaying V for the operator $H = Q(p) + V$.

To define the exceptional points we need the following notation: For $\omega \in \mathbb{R}^d$ we let $P_\perp(\omega) = I - |\omega\rangle\langle\omega|$ (defined in terms of inner product brackets).

Definition. Let $\lambda \in \mathbb{R}$ be given. The set of exceptional points $\Sigma_{\text{exc}}(\lambda)$ is the set of $\sigma \in (0, \infty)$ for which there exists $(\omega, \xi) \in S^{d-1} \times \mathbb{R}^d$ satisfying the equations

$$Q(\xi + i\sigma\omega) = \lambda, \tag{1.2a}$$

$$P_\perp(\omega)\nabla_\xi Q(\xi + i\sigma\omega) = 0. \tag{1.2b}$$

Another major subject of this paper is absence of super-exponentially decaying eigenfunctions (corresponding to the case $\sigma_c = \infty$), cf. [FHH201, VW, IS2]. We show absence of such states under somewhat strong decay conditions on the potential.

1.1. Results. Suppose $(H - \lambda)\phi = 0$, $\phi \in L^2$, with corresponding critical decay rate σ_c . Let $\text{Ran}Q = \{Q(\xi) | \xi \in \mathbb{R}^d\}$. Our main results read:

Theorem 1.1. *Under either of the following two conditions we can conclude that $\sigma_c > 0$:*

- 1) $\lambda \notin \text{Ran}Q$ and $V(x) = o(1)$ at infinity.
- 2) $\lambda \in \text{Ran}Q$ but λ is not a critical value of Q and in addition

$$\begin{aligned} \forall \alpha : \partial^\alpha V_1(x) &= o(|x|^{-|\alpha|}), \\ V_2(x) &= o(|x|^{-1}). \end{aligned}$$

Theorem 1.2. *Suppose $0 < \sigma_c < \infty$.*

- i) *If $V(x) = o(1)$ there exists $(\omega, \xi) \in S^{d-1} \times \mathbb{R}^d$ with*

$$Q(\xi + i\sigma_c\omega) = \lambda. \tag{1.3}$$

- ii) *If*

$$\begin{aligned} \forall \alpha : \partial^\alpha V_1(x) &= o(|x|^{-|\alpha|}), \\ V_2(x) &= o(|x|^{-1/2}), \end{aligned}$$

then $\sigma_c \in \Sigma_{\text{exc}}(\lambda)$.

Theorem 1.2 ii) gives stringent necessary conditions on a decay rate, namely that it belong to $\Sigma_{\text{exc}}(\lambda)$. To see that in certain situations *all* of the elements of $\Sigma_{\text{exc}}(\lambda)$ can occur as decay rates, see the discussion in Subsection 1.2 where we consider the family of Q 's which are polynomials in ξ^2 .

In a generic sense (see the remark following the theorem), the next result gives a more precise estimate on the decay of ϕ once we know $\sigma_c \in (0, \infty)$.

Theorem 1.3. *Suppose $0 < \sigma_c < \infty$. Suppose $\forall \alpha : \partial^\alpha V_1(x) = O(|x|^{-|\alpha|-\delta_1})$ and $V_2(x) = O(|x|^{-1/2-\delta_2})$ with $\delta_1, \delta_2 > 0$. Then either there exists $(\omega, \xi) \in S^{d-1} \times \mathbb{R}^d$ satisfying*

$$Q(\xi + i\sigma_c\omega) = \lambda \text{ and } \nabla_\xi Q(\xi + i\sigma_c\omega) = 0, \tag{1.4}$$

or for any $\epsilon \in (0, \epsilon')$ where $\epsilon' = \min(\delta_1, 2\delta_2, 1)$,

$$e^{\sigma_c(|x| - |x|^{1-\epsilon})} \phi \in L^2.$$

Note that (1.3) is necessary for $\sigma_c \in \Sigma_{\text{exc}}(\lambda)$ while (1.4) is sufficient. We give an example in Subsection 1.2 for which the $2d + 2$ real equations (1.4) (for $2d$ unknowns) do not have solutions in a generic sense. Whence for that example the second alternative of Theorem 1.3 is generic.

The following theorem eliminates the possibility of super-exponential decay at the expense of rather strong decay assumptions on the potential:

Theorem 1.4. *Suppose $V_2(x) = O(|x|^{-q/2-\delta})$ and $\partial^\alpha V_1(x) = O(|x|^{-(\delta+q+|\alpha|)/2})$, $1 \leq |\alpha| \leq q$, where $\delta > 0$. Then $\sigma_c < \infty$ unless $\phi = 0$.*

The restriction on the potentials in Theorem 1.4 is in general not optimal. In the special cases $Q(\xi) = \xi^2$ and $Q(\xi) = (\xi^2)^2$ we improve the bounds used to prove Theorem 1.4 to get better results in the next theorem. We prove this theorem in Subsection 9.4. There we use specific properties of the above polynomials for which our verification of the bounds appears very ad hoc. The main virtue of Theorem 1.4 is its generality.

Theorem 1.5. *Suppose $Q(\xi) = |\xi|^{2j}$, $j = 1$ or $j = 2$. Suppose $V_2(x) = O(|x|^{-\delta-j/2})$ and $\partial^\alpha V_1(x) = O(|x|^{-(\delta+j+|\alpha|)/2})$, $1 \leq |\alpha| \leq j$, where $\delta > 0$. Then $\sigma_c < \infty$ unless $\phi = 0$.*

In Lemma 9.1 we show optimality of the bound used to prove Theorem 1.5 for $(\xi^2)^2$. Whence a possible further improvement of the decay rates specified for $(\xi^2)^2$ would require a completely new method of proof.

Remarks 1.6. 1) For all our results we can allow V_2 to be complex-valued virtually without any complication in the proofs, however we need V_1 to be real-valued and λ to be real.

2) If $\lambda \notin \text{Ran}Q$ and $V(x) = o(1)$, Theorems 1.1 and 1.2 give

$$\sigma_c \geq \inf\{\sigma > 0 \mid \exists(\omega, \xi) \in S^{d-1} \times \mathbb{R}^d : Q(\xi + i\sigma\omega) = \lambda\}.$$

There is a different proof of this bound using a Combes -Thomas argument [CT].

3) The result for $Q(\xi) = \xi^2$ in Theorem 1.5 is well-known. See for example [FHH202, FHH203].

4) It is possible to treat some variable coefficient cases for most of our results. (We do not make these generalizations precise.) This possibility is due to the fact that most of our results are based on the general theory of pseudodifferential operators which is rather robust. Only Theorems 1.4 and 1.5 which are based on exact combinatorial formulas do not readily generalize to variable coefficient cases. In concrete situations as in Theorem 1.5 a perturbative argument works. Thus one can include classes of first and second order polynomials with variable coefficients for the examples ξ^2 and $(\xi^2)^2$, respectively. This follows readily by a little refinement of the improved bounds, so-called subelliptic estimates, see (9.25) and (9.26a).

5) Another potential direction of generalization concerns elliptic real-analytic dispersion relations (rather than elliptic polynomials), for example $Q(\xi) = (1 + |\xi|^2)^{q/2}$ for any real $q > 0$. Indeed we expect that our methods could yield versions of Theorems 1.1–1.3 for a general class of such symbols. This would require (omitting further details) a uniform analyticity radius say $\sigma_a > 0$ (in other words that there is an analytic extension of the symbol to a d -dimensional strip of width $2\sigma_a$) and conditions of at most polynomial growth and ellipticity (with constants being locally uniform in the imaginary part). Of course the hypothesis $\sigma_c < \sigma_a$ should be added to the corresponding versions of Theorems 1.2 and 1.3. See [MP2] for estimates leading to $\sigma_c > 0$ for a class of such dispersion relations under conditions overlapping the condition 2) of Theorem 1.1.

6) One way to think about the conditions (1.2a) and (1.2b) is the following: Write

$$Q(\xi + i\sigma\omega(x)) - \lambda = (X + iY)(\xi + i\sigma\omega(x)); \omega(x) = \hat{x} = x/|x|,$$

and look at the Hamiltonian $h(x, \xi) = X(\xi + i\sigma\omega(x))$. Due to the Cauchy-Riemann equations, for any Hamiltonian orbit (x, ξ) for h (with $x \neq 0$)

$$\begin{cases} d_\tau \omega = |x| \dot{\omega} &= P_\perp(\omega) \partial_\xi X(\xi + i\sigma\omega), \\ d_\tau \xi = |x| \dot{\xi} &= \sigma P_\perp(\omega) \partial_\xi Y(\xi + i\sigma\omega). \end{cases} \quad (1.5)$$

This is a reduced system of ordinary differential equations in the rescaled time τ . The conditions (1.2b) are exactly the conditions for a fixed point of the flow (1.5). In general $X(\xi + i\sigma\omega)$ is constant while $Y(\xi + i\sigma\omega)$ is growing for the flow (1.5).

1.2. Principal example, $Q(\xi) - \lambda = G(\xi^2)$. We aim at understanding the consequences of (1.2a) and (1.2b) for $\sigma > 0$ for the rotationally invariant case. Note first that for general Q these two equations are actually $2 + 2(d-1) = 2d$ real scalar equations for the $2d$ variables ξ, ω , and σ . This indicates that the set of solutions to the system of equations in general situations is discrete. However in the case of rotational invariance this is not true due to an overall rotational symmetry: If (ξ, ω, σ) is a solution then for any real orthogonal matrix R , $(R\xi, R\omega, \sigma)$ is also a solution. Now let us fix $\omega \in S^{d-1}$, and let $z = (\xi + i\sigma\omega)^2$. We have two equations:

$$\begin{aligned} G(z) &= 0, \\ P_\perp(\omega) \nabla_\xi Q(\xi + i\sigma\omega) &= 2G'(z) P_\perp(\omega) \xi = 0. \end{aligned}$$

If $P_\perp(\omega) \xi = 0$ then $\xi = \pm|\xi|\omega$ so that $G(z) = 0$ is the same as $G((\pm|\xi| + i\sigma)^2) = 0$. Note that for each pair of complex conjugate roots of G there will generally correspond two roots $\zeta = \pm|\xi| + i\sigma$ in the upper half plane of the polynomial $\tilde{G}(\zeta) := G(\zeta^2)$. On the other hand if $P_\perp(\omega) \xi \neq 0$ then we have the two equations $G(z) = G'(z) = 0$ which require G to have a multiple zero. If Q has degree q this can only happen at at most $q/2 - 1$ values of λ . If λ is not one of these at most $q/2 - 1$ possible real numbers there are at most $q/2$ exceptional numbers σ_c . In the case of $G(z) = z^2 - \lambda$, involving the bilaplacian, if $\lambda \neq 0$ there is exactly one solution with positive σ . Namely $\sigma = \lambda^{1/4}$ if $\lambda > 0$ and $\sigma = (-\lambda/4)^{1/4}$ if $\lambda < 0$. On the other hand by the construction below each of these cases is realized by a compact support potential.

In the situation of Theorem 1.3 where we have $Q(\xi + i\sigma\omega) = \lambda$ and $\nabla Q(\xi + i\sigma\omega) = 0$, either we are in the non-generic case $G(z) = G'(z) = 0$ or we have $\xi + i\sigma\omega = 0$, an impossible situation since $\sigma > 0$.

We remark that as in the N -body problem where for a fixed negative eigenvalue there are typically many exponential decay rates possible determined by the thresholds for the problem, we have a similar situation for $H = Q(p) + V(x)$ even for V of compact support.

Let us for any $\lambda \in \mathbb{R}$ consider any zero $z \in \mathbb{R} \setminus [0, \infty)$ of the function G . There is a unique $k \in \mathbb{C}$ with $\sigma := \text{Im } k > 0$ and $z = k^2$, and according to the above discussion $\sigma \in \Sigma_{\text{exc}}(\lambda)$. We will display a real $V \in C_c^\infty(\mathbb{R}^d)$ and a function $\phi \in L^2$ satisfying $(G(-\Delta) + V)\phi = 0$ with critical decay rate $\sigma_c = \sigma$. Letting K be the integral kernel of $(-\Delta - z)^{-1}$ the function $\tilde{\phi}(x) = \text{Re}K(x, 0)$ satisfies $G(-\Delta)\tilde{\phi} = 0$ for $x \neq 0$. Since $\tilde{\phi}(x) > 0$ for small $|x|$ (see [AS, p. 360] and [T, p. 232–233]) we can modify $\tilde{\phi}$ there to obtain a function ϕ with $V := G(-\Delta)\phi/\phi$ smooth with compact support. To carry out this modification choose R so that $\tilde{\phi} > 0$ for $0 < |x| < R$. Let $\chi \in C_c^\infty(\mathbb{R}^d)$ with $0 \leq \chi \leq 1$ and $\chi = 1$ if $0 \leq |x| < R/2$ and $\chi = 0$ if $|x| > 3R/4$.

Let $\phi = \chi + (1 - \chi)\tilde{\phi}$. Then ϕ is smooth and positive for $|x| < R$ while $G(-\Delta)\phi$ has support in $|x| \leq 3R/4$. Thus indeed V is real, smooth and compactly supported. Clearly $\sigma_c = \sigma$ (see [AS, p. 364] and [T, p. 232–233]).

These considerations show that for Q any elliptic polynomial in ξ^2 , except for at most $q/2 - 1$ real λ 's, $\sigma \in \Sigma_{\text{exc}}(\lambda)$ is sufficient for σ to be the critical decay rate of an eigenfunction with eigenvalue λ and for some compactly supported real potential V . The converse statement, necessity, is stated for a more general Q in Theorem 1.2 ii).

1.3. Local critical decay rate. For an eigenfunction ϕ we define the *local critical decay rate* in direction $\omega \in S^{d-1}$ as

$$\sigma_{\text{loc}}(\omega) = \sup\{\sigma \geq 0 \mid e^{\sigma|x|}\chi_\omega(\hat{x})\phi \in L^2 \\ \text{for some } \chi_\omega \in C(S^{d-1}), \chi_\omega(\omega) = 1\}$$

Here $\hat{x} = x/|x|$, and thus χ_ω is a conical localization factor in the direction of ω . For this concept of decay the Euclidean structure of \mathbb{R}^d plays the role of normalization only. Thus if we define $\sigma_{\text{loc}}(x) = \sigma_{\text{loc}}(\hat{x})|x|$, this quantity is independent of the Euclidean structure. On the other hand the concept of exponential decay studied in this paper clearly is fundamentally linked to the Euclidean structure of the underlying space. One can view σ_{loc} as a quantity carrying some rough information on asymptotics of the given eigenfunction. For partial results on finer asymptotics of the Green's function of $Q(p)$ we refer to [Ag].

In our paper [HS] we prove for $d \geq 2$ and $Q(\xi)$ rotation invariant (note that this particular model is born with Euclidean structure) that the local critical decay rate is an angle-independent constant and that this constant coincides with the (global) critical decay rate:

Theorem 1.7. *[Rotationally invariant case, $Q(\xi) - \lambda = G(\xi^2)$] Suppose $d \geq 2$ and that V_1 and V_2 fulfill the conditions of Theorem 1.2 ii). For $H\phi = \lambda\phi$, $\sigma_c \in (0, \infty)$ and λ not in a set of at most $q/2 - 1$ energies:*

$$\text{For all } \omega \in S^{d-1} : \quad \sigma_{\text{loc}}(\omega) = \sigma_c.$$

The excluded set of at most $q/2 - 1$ energies is given as in Subsection 1.2 and, as we showed there, σ_c belongs to a set of at most $q/2$ elements.

For a general real elliptic polynomial Q the local critical decay rate for an eigenfunction $H\phi = \lambda\phi$, $\sigma_c \in (0, \infty)$, is in some situations determined algebraically as follows: For fixed $\lambda \in \mathbb{R}$ and $\omega \in S^{d-1}$ consider the equations

$$Q(\xi + i\eta) = \lambda, \tag{1.6a}$$

$$\nabla_\xi Q(\xi + i\eta) = \beta\omega, \tag{1.6b}$$

in the variables $(\xi, \eta, \beta) \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{C}$. Note that it is only the direction of ω that matters for the solvability of this system of equations. Whence it may be viewed as being independent of the Euclidean structure of \mathbb{R}^d , and in this sense being different from the system of equations (1.2a) and (1.2b). This will be discussed more fully in [HS].

In some situations the following holds for a given eigenfunction with eigenvalue λ : There exists a solution to the equations (1.6a) and (1.6b) such that

$$\sigma_{\text{loc}}(\omega) = \eta \cdot \omega. \tag{1.6c}$$

A main issue of [HS] is a detailed examination of this recipe. Clearly, to the extent it is valid, the assertion is an analogue of Theorem 1.2 ii) for the notion of local critical decay rate. We note that Theorem 1.7 is a particular example of its validity.

1.4. Notation and some calculus considerations. We shall use the Weyl calculus for symbols in $S(m, g)$ where the weight m may vary but the metric will be

$$g = \langle x \rangle^{-2} dx^2 + \langle \xi \rangle^{-2} d\xi^2.$$

Here and henceforth $\langle x \rangle = (1 + |x|^2)^{1/2}$ and similarly with $x \rightarrow \xi$; let also $\hat{x} = x/|x|$. See [Hö, Chapt. XVIII] for an exposition of the Weyl calculus including the results stated below and some additional ones in Subsection 3.1. Recalling $q = \text{degree}(Q)$ obviously $Q \in S(\langle \xi \rangle^q, g)$. In the bulk of this paper we shall in fact only use weights of the form $m = \langle x \rangle^s \langle \xi \rangle^t$, $s, t \in \mathbb{R}$. This standard class of symbols is associated to a well-functioning calculus, in particular one for which the ‘‘Planck constant’’ is $\langle x \rangle^{-1} \langle \xi \rangle^{-1}$. We use the notation $\text{Op}^w(a)$ for the Weyl quantization of a symbol a .

Recall the L^2 -boundedness result [Hö, Theorem 18.6.3] (alternatively see [D, L]), here exemplified as

$$a \in S(1, g) \Rightarrow \|\text{Op}^w(a)\| \leq C, \quad (1.7a)$$

where $C \geq 0$ can be chosen independently of a from any bounded family of symbols in $S(1, g)$. A family of such symbols is also said to be uniformly in $S(1, g)$. We shall use similar terminologies for symbols in $S(m, g)$. Whence a family $\{a_i \in S(m, g) | i \in I\}$ is *uniformly* (or *bounded*) in $S(m, g)$ if for all $\alpha, \beta \in \mathbb{N}_0^d$ there exists a constant $C \geq 0$ being independent of $i \in I$ such that

$$|\partial_x^\alpha \partial_\xi^\beta a_i(x, \xi)| \leq C m(x, \xi) \langle x \rangle^{-|\alpha|} \langle \xi \rangle^{-|\beta|}.$$

By the so-called sharp Gårding inequality (cf. [Hö, Theorem 18.6.7] and [D, L])

$$a \in S(\langle x \rangle \langle \xi \rangle, g), a \geq 0 \Rightarrow \text{Op}^w(a) \geq -C, \quad (1.7b)$$

where $C \geq 0$ can be chosen independently of a from any bounded family of such symbols. The stronger estimate, the so-called Fefferman-Phong inequality, cf. [Hö, Theorem 18.6.8] and [D, L], is not needed for our analysis.

For our applications of (1.7a) and (1.7b) the relevant families of symbols will be given in terms of real parameters. A typical and useful example of such a family of symbols is given as

$$a = a_k(x, \xi) = \langle x \rangle (1 + \langle x \rangle/k)^{-1}; \quad k \in \mathbb{N}.$$

This family of bounded symbols is uniformly in $S(\langle x \rangle, g)$.

Let χ_1 and χ_2 denote smooth non-negative functions on \mathbb{R} with $\chi_1(t) = 1$ for $t \leq 1$, $\chi_2(t) = 0$ for $t \geq 2$ and

$$\chi_1^2 + \chi_2^2 = 1. \quad (1.8)$$

For any $\kappa > 0$ we define $\chi(t \leq \kappa) = \chi_1(t/\kappa)$ and $\chi(t \geq \kappa) = \chi_2(t/\kappa)$.

In this paper bounding constants are typically denoted by c, C or C_j . They may vary from line to line. For any operator A (or form) we abbreviate the inner product $\langle \psi, A\psi \rangle = \langle A \rangle_\psi$.

1.4.1. *Distorted* $|x|$. We are going to use two qualitatively different distorted versions of the function $|x|$ on \mathbb{R}^d . The first one is

$$r(x) = r_1(x) = \langle x \rangle. \quad (1.9a)$$

The second one is given in terms of a parameter $\epsilon \in (0, 1)$ as

$$r(x) = r_\epsilon(x) = \langle x \rangle - \langle x \rangle^{1-\epsilon} + 1. \quad (1.9b)$$

Note that for all $\epsilon \in (0, 1]$ the function $r_\epsilon \geq 1$, is strictly convex and

$$r_\epsilon(x)/|x| = 1 - |x|^{-\epsilon} + O(|x|^{-1}). \quad (1.10)$$

However while r_1 tends to be degenerately convex at infinity (just as $|x|$), this deficiency appears somewhat cured for r_ϵ , $\epsilon \in (0, 1)$ (in particular in the regime where ϵ is small). As a symbol r is elliptic in $S(\langle x \rangle, g)$. We shall use the notation $\omega = \omega(x) = \text{grad } r$. For $\epsilon \in (0, 1)$ the function r is used in [RT] in a different context, and yet another application is given in [IS1].

2. IDEAS OF PROOF OF THEOREMS 1.2 AND 1.3

Consider the function r given by either (1.9a) or (1.9b).

We introduce for $\sigma \geq 0$

$$Q(\xi + i\sigma\omega(x)) - \lambda = (X + iY)(\xi + i\sigma\omega(x)).$$

This is to leading order the symbol of

$$e^{\sigma r} \{Q(p) - \lambda\} e^{-\sigma r} = Q(p + i\sigma\omega(x)) - \lambda.$$

Also we introduce the distorted energy surface

$$S_{\sigma, \lambda} = \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d | Q(\xi + i\sigma\omega(x)) = \lambda\} = \{X = Y = 0\}. \quad (2.1)$$

Now suppose ϕ is an eigenfunction with eigenvalue λ , i.e. $(H - \lambda)\phi = 0$. Suppose that $\phi_\sigma := e^{\sigma r} \phi \in L^2$ for some small $\sigma > 0$ (We do not justify this assumption here. It is proved in Section 8 under the assumptions of Theorem 1.1.) So we consider an eigenfunction ϕ with $\phi_{\sigma_0} \in L^2$ for some $\sigma_0 > 0$ and want to derive a priori bounds of ϕ_σ for $\sigma < \sigma_c$. See (2.7) for an example of such bound.

The result Theorem 1.2 i) which can be interpreted as an energy estimate will not be discussed here. On the other hand Theorem 1.2 ii) and Theorem 1.3 are strongly based on (strict) positivity of a certain commutator to be explained.

Introducing the shorthand notation

$$\eta = \sigma\omega(x) \text{ and } \zeta = \xi + i\eta,$$

the Cauchy-Riemann equations for $\zeta \rightarrow Q(\zeta)$ and the chain rule allow us to calculate the Poisson bracket

$$\sigma^{-1} \{X, Y\} = \partial_\xi X \omega'(x) \partial_\xi^T X + \partial_\xi Y \omega'(x) \partial_\xi^T Y. \quad (2.2)$$

Whence in particular

$$\{X, Y\} \geq 0. \quad (2.3)$$

We propose to consider the *conjugate operator* A_c with Weyl symbol

$$a_c = rY(\zeta) = rY(\xi + i\sigma\omega(x)).$$

Consider

$$i[Q(p), e^{\sigma r} A_c e^{\sigma r}] = e^{\sigma r} (i[\tilde{X}, A_c] + 2\text{Re}(\tilde{Y}A)) e^{\sigma r} = 2e^{\sigma r} \text{Im}(A_c(\tilde{X} + i\tilde{Y})) e^{\sigma r},$$

where $\tilde{X} = \operatorname{Re}(e^{\sigma r} Q(p) e^{-\sigma r}) - \lambda$ and $\tilde{Y} = \operatorname{Im}(e^{\sigma r} Q(p) e^{-\sigma r})$.

To leading order the symbol of the operator between exponentials to the right has symbol

$$r\{X, Y\} + 2rY^2 + \{X, r\}Y.$$

Note that the second term is also non-negative.

In the remaining part of this section we only discuss the proof of Theorem 1.3.

Let us note that if $\sigma > 0$ a sufficient condition for $S_{\sigma, \lambda}$ to be a codimension 2 submanifold of \mathbb{R}^{2d} is

$$\nabla_{\xi} Q(\xi + i\sigma\omega(x)) \neq 0 \text{ for all } (x, \xi) \in S_{\sigma, \lambda}. \quad (2.4)$$

This is due to the Cauchy-Riemann equations.

Under the regularity condition (2.4) there is a chance of deriving some positivity from (2.2), gaining positivity from the first term. In fact, discussing here only $r = r_{\epsilon}$, a slight strengthening of the regularity condition (2.4) yields the following bounds in a neighbourhood of $S_{\sigma, \lambda}$,

$$\begin{aligned} r\{X, Y\} &\geq 3cr^{-\epsilon}, \\ \{X, r\}Y &\geq -rY^2 - Cr^{-1}, \end{aligned}$$

and therefore also

$$r\{X, Y\} + 2rY^2 + \{X, r\}Y \geq 2cr^{-\epsilon} + rY^2. \quad (2.5)$$

Next by using a proper energy cut-off the bound (2.5) should be persistent under quantization, cf. (1.7b). Along this line of thinking we shall in fact derive the bound

$$c\|r^{-\epsilon/2}\phi_{\sigma}\|^2 \leq -\langle i[V, A_c] \rangle_{\phi_{\sigma}} - \|r^{1/2}\tilde{Y}\phi_{\sigma}\|^2 + C\|\phi\|^2. \quad (2.6)$$

Now we insert the splitting $V = V_1 + V_2$ of Theorem 1.3 into the first term to the right. Assuming $\epsilon < \delta_1$ we can estimate the contribution from V_1 by doing the commutator. Assuming also $\frac{1}{2}(1 + \epsilon) < 1/2 + \delta_2$ we can estimate the contribution from V_2 by undoing the commutator using the second term to the right. As a result we can convert (2.6) into

$$\|r^{-\epsilon/2}\phi_{\sigma}\|^2 \leq C\|\phi\|^2. \quad (2.7)$$

Finally by taking $\sigma \nearrow \sigma_c$ in (2.7) and then invoking (1.10) we obtain the refined exponential upper bound of Theorem 1.3.

3. PRELIMINARIES

The goal of this section is to give more details on the calculus of pseudodifferential operators and to show an exponentially weighted elliptic estimate for the operator $Q(p)$.

3.1. Calculus of pseudodifferential operators. We supplement Subsection 1.4 with various standard facts for the calculus of pseudodifferential operators, see for example [Hö, Chapt. XVIII] for details. The metric and weight functions below are given as those specified in Subsection 1.4.

First we have chosen (for convenience) to work in the framework of Weyl quantization. Recall

$$\text{Op}^w(a)u(x) = (2\pi)^{-d} \iint e^{i(x-y)\cdot\xi} a((x+y)/2, \xi) u(y) dy d\xi.$$

The (left) Kohn-Nirenberg quantization would have been another option. It is defined by

$$\text{Op}^l(b)u(x) = (2\pi)^{-d} \iint e^{i(x-y)\cdot\xi} b(x, \xi) u(y) dy d\xi.$$

Now defining $a = e^{-ip_x \cdot p_\xi / 2} b$

$$\text{Op}^w(a) = \text{Op}^l(b), \quad (3.1)$$

and this relation defines an isomorphism on $S(m, g)$ which (together with its inverse) takes any bounded family of symbols in $S(m, g)$ into a bounded family of symbols in $S(m, g)$, cf. [Hö, Theorem 18.5.10]. In the natural semi-norm topology on $S(m, g)$ this isomorphism is bi-continuous.

Second the composition rule for pseudodifferential operators (adapted to our context) reads as follows, cf. [Hö, Theorem 18.5.4]. Let $h = \langle x \rangle^{-1} \langle \xi \rangle^{-1}$. Suppose $a_1 \in S(m_1, g)$ and $a_2 \in S(m_2, g)$. Then $\text{Op}^w(a_1)\text{Op}^w(a_2) = \text{Op}^w(b)$ with $b \in S(m_1 m_2, g)$, and asymptotically $b \equiv \sum_{j=0}^{\infty} b_j(x, \xi)$ with

$$b_j(x, \xi) \in S(h^{-j} m_1 m_2, g)$$

given by

$$b_j(x, \xi) = 2^{-j} i^j \sum_{|\alpha+\beta|=j} \frac{(-1)^{|\alpha|}}{\alpha! \beta!} (\partial_\xi^\alpha \partial_x^\beta a_1) (\partial_\xi^\beta \partial_x^\alpha a_2). \quad (3.2)$$

Here ‘asymptotically’ means that for all $n \in \mathbb{N}_0$ we have

$$b - \sum_{j=0}^n b_j \in S(h^{-n-1} m_1 m_2, g).$$

If a_1 and a_2 belong to bounded families in $S(m_1, g)$ and $S(m_2, g)$, respectively, the same is true for this remainder in $S(h^{-(n+1)} m_1 m_2, g)$; this is a consequence of continuity estimates. It is convenient at this point to introduce the notation

$$\Psi(m, g) = \{\text{Op}^w(a) \mid a \in S(m, g)\}.$$

Note that (3.2) yields (in terms of the Poisson bracket)

$$b_0 = a_1 a_2 \text{ and } b_1 = -\frac{i}{2} \{a_1, a_2\}, \quad (3.3)$$

and whence,

$$i[\text{Op}^w(a_1), \text{Op}^w(a_2)] - \text{Op}^w(\{a_1, a_2\}) \in \Psi(h^{-3} m_1 m_2, g). \quad (3.4)$$

We shall use (1.7b) on the following more general form (which in turn is an easy consequence of the bounds (1.7a) and (1.7b) and the composition rule).

$$a \in S(\langle x \rangle^{1+2s} \langle \xi \rangle^{1+t}, g), a \geq 0 \Rightarrow \text{Op}^w(a) \geq -C \langle x \rangle^s \langle p \rangle^t \langle x \rangle^s, \quad (3.5)$$

where $C = C(s, t, \mathcal{F}) \geq 0$ can be chosen independently of a from any bounded family $\mathcal{F} \subset S(\langle x \rangle^{1+2s} \langle \xi \rangle^{1+t}, g)$.

3.2. Exponentially conjugated operator. Now as a first step to relate these calculus considerations with our problems let us consider any real symbol $f = f(x) \in S(\langle x \rangle, g)$ and the operator

$$A := Q(p + i\nabla f).$$

Since the components $p_j + i\partial_j f$, $j = 1, \dots, d$, commute obviously A is well-defined as an operator on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$; in fact with this interpretation $A = e^f Q(p) e^{-f}$. Moreover since $p_j + i\partial_j f$ has Weyl symbol $\xi_j + i\partial_j f \in S(\langle \xi \rangle, g)$ indeed by the above calculus A has Weyl symbol $a \in S(\langle \xi \rangle^q, g)$. By symmetry similar considerations work for the formal adjoint operator $Q(p - i\nabla f)$. Whence by the standard procedure of extending pseudodifferential operators we can consider A as an operator on the space of tempered distributions (by definition given as the space of continuous, complex conjugate linear functionals on the Schwartz space) by the recipe

$$\langle \phi, Al \rangle = \langle Q(p - i\nabla f)\phi, l \rangle; \quad \phi \in \mathcal{S}(\mathbb{R}^d), l \in \mathcal{S}'(\mathbb{R}^d).$$

Let H^q be the standard Sobolev space of order q ,

$$H^q = \{\psi \in L^2 \mid \partial^\alpha \psi \in L^2 \text{ for } |\alpha| \leq q\}.$$

By the L^2 -continuity bound (1.7a) we see that $A : H^q \rightarrow L^2$ is bounded. We note, although this will not be needed, that the symbol a is a polynomial in ξ (in fact this polynomial can be computed explicitly). One way to see this is to move all components of p to the right yielding that $A = \text{Op}^1(b)$ with b being a polynomial of degree q . Then we apply (3.1) and see that also a is a polynomial of degree q . For our purposes the following approximation suffices.

$$a(x, \xi) \equiv Q(\xi + i\nabla f) \pmod{S(\langle x \rangle^{-1} \langle \xi \rangle^{q-2}, g)}. \quad (3.6)$$

The right hand side is the polynomial

$$Q(\xi + i\nabla f) = \Sigma_\alpha(\alpha!)^{-1} (i\nabla f(x))^\alpha Q^{(\alpha)}(\xi). \quad (3.7)$$

Whence in particular $\text{Im } a, \text{Re } a - Q(\xi) \in S(\langle \xi \rangle^{q-1}, g)$, and therefore in turn a and $\text{Re } a$ are elliptic symbols in $S(\langle \xi \rangle^q, g)$. Moreover writing

$$\begin{aligned} Q(\xi + i\nabla f) &= \text{Re } Q(\cdot) + i\text{Im } Q(\cdot) = X + iY, \\ A &= \text{Op}^w(\text{Re } a) + i\text{Op}^w(\text{Im } a) = \tilde{X} + i\tilde{Y}, \end{aligned}$$

which is consistent with Section 2 except for the constant λ used there, it follows from (3.6) that

$$\tilde{X} - \text{Op}^w(X) \in \Psi(\langle x \rangle^{-1} \langle \xi \rangle^{q-2}, g), \quad (3.8a)$$

$$\tilde{Y} - \text{Op}^w(Y) \in \Psi(\langle x \rangle^{-1} \langle \xi \rangle^{q-2}, g). \quad (3.8b)$$

3.3. Exponentially weighted Sobolev estimate. We shall prove the following for our elliptic polynomial Q .

Lemma 3.1. *Consider a real symbol $f = f(x) \in S(\langle x \rangle, g)$ and $\psi \in H^q$. Suppose $e^f \psi \in L^2$ and $e^f Q(p)\psi \in L^2$. Then $e^f \psi \in H^q$ and*

$$Ae^f \psi = Q(p + i\nabla f)e^f \psi = e^f Q(p)\psi. \quad (3.9)$$

Moreover there exists $C \geq 0$ such that

$$\|e^f \psi\|_{H^q} \leq C(\|e^f Q(p)\psi\| + \|e^f \psi\|), \quad (3.10)$$

and C can be chosen independent of f 's from any bounded subset of $S(\langle x \rangle, g)$.

Proof. Introduce the family of bounded symbols

$$f_k(x) = f(x)(1 + if(x)/k)^{-1}; \quad k \in \mathbb{N}.$$

Clearly $e^{f_k}\psi \in H^q$ and

$$Q(p + i\nabla f_k)e^{f_k}\psi = e^{f_k}Q(p)\psi. \quad (3.11)$$

We take L^2 -inner product with any $\phi \in \mathcal{S}(\mathbb{R}^d)$ and let $k \rightarrow \infty$ using the dominating convergence theorem. This yields

$$\langle Q(p - i\nabla f)\phi, e^f\psi \rangle = \langle \phi, e^fQ(p)\psi \rangle,$$

and therefore in turn (3.9) as an identity in $\mathcal{S}'(\mathbb{R}^d)$.

It remains to show that (3.9) implies that $e^f\psi \in H^q$ and to show the estimate (3.10) with a 'uniform' constant. We use the standard procedure. For a big constant $K > 0$ the symbol

$$b(x, \xi) := (Q(\xi + i\nabla f(x)) + iK)^{-1} \in S(\langle \xi \rangle^{-q}, g). \quad (3.12)$$

Letting $B = \text{Op}^w(b)$

$$B(Q(p + i\nabla f) + iK) = I + R, \quad (3.13)$$

where $R \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^{-1}, g)$. Whence

$$B_q(Q(p + i\nabla f) + iK) = I + R_q, \quad (3.14)$$

where $B_q = \sum_{0 \leq j \leq q-1} (-R)^j B$ and $R_q = (-1)^{q-1} R^q$. We have $B_q, R_q \in \Psi(\langle \xi \rangle^{-q}, g)$, so by applying (3.14) to (3.9) we obtain

$$e^f\psi = B_q e^f(Q(p)\psi + iK\psi) - R_q e^f\psi \in H^q.$$

Obviously the estimate (3.10) is a consequence of this formula. If f belongs to a bounded subset of $S(\langle x \rangle, g)$ the constant K can be chosen independent of the individual elements of the family. So by using the continuity bounds of the calculus the constant C in (3.10) can be chosen independent of f 's from any bounded subset of $S(\langle x \rangle, g)$. \square

3.4. More elliptic estimates. The ellipticity property of a and $\text{Re } a$, where

$$A = \text{Op}^w(a) = Q(p + i\nabla f) = \tilde{X} + i\tilde{Y},$$

yields the following bounds.

Lemma 3.2. *Let $r = r_\epsilon$, $\epsilon \in (0, 1]$, be given as in Subsection 1.4. For all real symbols $f = f(x) \in S(\langle x \rangle, g)$ and $t \in \mathbb{R}$*

$$r^t \langle p \rangle^{2q} r^t \leq C(\tilde{X} r^{2t} \tilde{X} + r^{2t}), \quad (3.15a)$$

$$r^t \langle p \rangle^{2q} r^t \leq C(A^* r^{2t} A + r^{2t}), \quad (3.15b)$$

where the constant $C = C(t, \mathcal{F}) \geq 0$ can be chosen independently of f from any bounded family $\mathcal{F} \subset S(\langle x \rangle, g)$.

Proof. We mimic the proof of the last part of Lemma 3.1 showing only (3.15a). Introduce for $K > 0$ big enough the symbol $b = (\operatorname{Re} a + iK)^{-1} \in S(\langle \xi \rangle^{-q}, g)$, cf. (3.12). In terms of $B := \operatorname{Op}^w(b)$ and $A_K := \tilde{X} + iK$ we define

$$R = BA_K - I \in \Psi(\langle \xi \rangle^{-1}, g),$$

cf. (3.13). By a similar truncation of the Neumann series of $(I + R)^{-1}$ we obtain the following analogue of (3.14):

$$B_{2q}A_K - I = R_{2q} \in \Psi(\langle \xi \rangle^{-2q}, g). \quad (3.16)$$

By the calculus

$$B_{2q}^* r^t \langle p \rangle^{2q} r^t B_{2q} \leq Cr^{2t}.$$

We multiply by A_K^* and A_K from the left and from the right, respectively, yielding

$$(I + R_{2q}^*) r^t \langle p \rangle^{2q} r^t (I + R_{2q}) \leq CA_K^* r^{2t} A_K.$$

The left hand side equals

$$r^t \langle p \rangle^{2q} r^t \quad \text{mod } \psi(\langle x \rangle^{2t}, g).$$

To the right we insert $A_K = \tilde{X} + iK$ and use

$$(\tilde{X} - iK)r^{2t}(\tilde{X} + iK) \leq 2\tilde{X}r^{2t}\tilde{X} + 2K^2r^{2t},$$

which follows from the Cauchy-Schwarz inequality. We have proved (3.15a). The uniformity property of constants follows as before. \square

3.4.1. *Application of Lemma 3.2 and discussion.* Note that (3.8a) and (3.8b) imply

$$i[\tilde{X}, \tilde{Y}] - \operatorname{Op}^w(\{X, Y\}) \in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{2q-3}, g).$$

Computing the bracket by the Cauchy-Riemann equations yields

$$i[\tilde{X}, \tilde{Y}] - \operatorname{Op}^w(\partial_\xi X(\nabla^2 f)(x)\partial_\xi^T X + \partial_\xi Y(\nabla^2 f)(x)\partial_\xi^T Y) \in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{2q-3}, g). \quad (3.17)$$

By combining (3.5) and (3.17) we obtain that for any *convex* $f = f(x) \in S(\langle x \rangle, g)$

$$i[\tilde{X}, \tilde{Y}] \geq \operatorname{Op}^w(b); \quad b \in S(\langle x \rangle^{-2} \langle \xi \rangle^{2q-3}, g), \quad (3.18)$$

while without convexity we only have the obvious lower bound deducible from

$$i[\tilde{X}, \tilde{Y}] \in \Psi(\langle x \rangle^{-1} \langle \xi \rangle^{2q-2}, g),$$

for example written

$$i[\tilde{X}, \tilde{Y}] \geq -Cr^{-1/2} \langle p \rangle^{2q-2} r^{-1/2}. \quad (3.19)$$

Some of the energy bounds we are going to use can be improved using (3.18) rather than (3.19). However since the convexity property is not fulfilled for all cases we only prove the weaker ones using (3.19). By applying Lemma 3.2 to the right hand side of (3.19) we obtain the following rough bounds: For all $s \in \mathbb{R}$ there exists $n \in \mathbb{N}$ such that

$$\begin{aligned} r^s i[\tilde{X}, \tilde{Y}] r^s &\geq -C_1 r^{s-1/2} \langle p \rangle^{2q-2} r^{s-1/2} \\ &\geq -C_2 (A^* r^{2s-1} \tilde{A} + r^{2s-1}) \\ &\geq -A^* r^{2s} A - C_3 A^* \chi^2(r \leq n) A - C_2 r^{2s-1}. \end{aligned} \quad (3.20)$$

Note that the last estimate is immediate from (1.8). As before the constants can be chosen independently of f from any bounded family $\mathcal{F} \subset S(\langle x \rangle, g)$.

4. A PRIORI ENERGY LOCALIZATION

This section contains various preliminary Sobolev and energy bounds valid for any eigenfunction ϕ , $(H - \lambda)\phi = 0$, with $\sigma_c > 0$. In Subsections 4.1 and 4.2 these are, more precisely, a priori bounds of $\phi_\sigma := e^{\sigma r}\phi$ for $\sigma \in [0, \sigma_c)$ where r is the function given by either (1.9a) or (1.9b). The bounds are uniform in σ varying in any bounded subset of $[0, \sigma_c)$. In Subsection 4.3 we establish uniform bounds using a certain (non-convex) parameter-dependent approximation of this kind of phase factor. Throughout this section we shall only need boundedness of V (i.e. decay assumptions will not be needed).

4.1. Sobolev regularity bounds. Let us note that

$$\forall \sigma \in [0, \sigma_c) \forall s \in \mathbb{R} : \phi_\sigma \in r^{-s}H^q =: H_s^q, \quad (4.1)$$

where H^q is the Sobolev space of order q . This follows from Lemma 3.1 applied with $f(r) = \sigma r + s \ln r$ and $\psi = \phi$. By (3.10) we can estimate

$$\|e^f \phi\|_{H^q} \leq C(\|e^f(\lambda - V)\phi\| + \|e^f \phi\|). \quad (4.2)$$

In the natural norm-topology $\mathcal{S}(\mathbb{R}^d)$ in dense in H_s^q . This property will tacitly be used to extend various form estimates (in particular involving commutator forms).

4.2. Refined energy bounds. With $f(r) = \sigma r$ we write

$$Q(p + i\nabla f) - \lambda = A = \tilde{X} + i\tilde{Y},$$

which is consistent with Section 3 except for the constant λ (not appearing there). This small discrepancy is resolved by applying Section 3 to $Q - \lambda$ rather than to Q .

Due to (4.1) we can calculate for $s \in \mathbb{R}$, on the one hand

$$\|r^s A \phi_\sigma\|^2 = T - 2\text{Im} \langle \tilde{X} r^{2s} \tilde{Y} \rangle_{\phi_\sigma}; \quad T = \|r^s \tilde{X} \phi_\sigma\|^2 + \|r^s \tilde{Y} \phi_\sigma\|^2, \quad (4.3a)$$

while on the other hand, cf. (3.9),

$$\|r^s A \phi_\sigma\|^2 = \|r^s V \phi_\sigma\|^2. \quad (4.3b)$$

The combination will lead to the useful bound (4.5) below. First let us note that for all $\kappa > 0$

$$\|\chi(r \leq n) A \phi_\sigma\|^2 = \|\chi(r \leq n) V \phi_\sigma\|^2 \leq C \|V \phi\|^2. \quad (4.4)$$

We need to examine the last term to the right in (4.3a). We use the Cauchy-Schwarz inequality in the first step bounding

$$\begin{aligned} & -2\text{Im} \langle \tilde{X} r^{2s} \tilde{Y} \rangle_{\phi_\sigma} - \langle i[\tilde{X}, \tilde{Y}] \rangle_{r^s \phi_\sigma} \\ & \geq -\frac{1}{2}T - C_1 \|\langle p \rangle^q r^{s-1} \phi_\sigma\|^2 \\ & \geq -\frac{1}{2}T - C_2 (\|r^{s-1} A \phi_\sigma\|^2 + \|r^{s-1} \phi_\sigma\|^2) \quad (\text{by (3.15b)}) \\ & \geq -\frac{1}{2}T - \|r^s A \phi_\sigma\|^2 - C_3 \|\chi(r \leq n) A \phi_\sigma\|^2 - C_2 \|r^{s-1} \phi_\sigma\|^2 \quad (\text{by (3.20)}) \\ & \geq -\frac{1}{2}T - \|r^s A \phi_\sigma\|^2 - C_4 \|V \phi\|^2 - C_2 \|r^{s-1} \phi_\sigma\|^2 \quad (\text{by (4.4)}). \end{aligned}$$

With the rough bound (3.20) and (4.4) we obtain

$$\langle i[\tilde{X}, \tilde{Y}] \rangle_{r^s \phi_\sigma} \geq -\|r^s A \phi_\sigma\|^2 - C_1 \|r^{s-1/2} \phi_\sigma\|^2 - C_2 \|V \phi\|^2.$$

In combination with (4.3a) these bounds yield

$$3\|r^s A \phi_\sigma\|^2 \geq \frac{1}{2}T - C_1 \|r^{s-1/2} \phi_\sigma\|^2 - C_2 \|V \phi\|^2,$$

and therefore by (4.3b) that

$$\|r^s \tilde{Y} \phi_\sigma\|^2 + \|r^s \tilde{X} \phi_\sigma\|^2 \leq 6 \|r^s V \phi_\sigma\|^2 + C \|r^{s-1/2} \phi_\sigma\|^2 + C \|V \phi\|^2. \quad (4.5)$$

Here $C > 0$ can be chosen independent of σ in any bounded subset of $[0, \sigma_c)$.

We have a related (actually on the formal level somewhat weaker) energy bound to be discussed next. By definition we write

$$Q(\xi + i\nabla f) - \lambda = X + iY.$$

Recalling the quadratic decomposition of unity (1.8) we introduce for any $\kappa > 0$ the symbol

$$\chi_- = \chi(X^2 + Y^2 \leq \kappa),$$

where we have suppressed the dependence on κ , and similarly for χ_+ . Thus we are going to use (1.8) for κ -dependent partition functions. Let correspondingly

$$\tilde{\chi}_\pm = \text{Op}^w(\chi_\pm).$$

Here obviously the subscript tilde refers to the exact Weyl quantization. For comparison $\tilde{X} + i\tilde{Y} \approx \text{Op}^w(X + iY)$ only. The precise meaning of this approximation is given in (3.8a) and (3.8b). It will be used in the proof of the following result.

Lemma 4.1. *For all $\kappa > 0$ and ϕ_σ as above*

$$\|\langle p \rangle^q \tilde{\chi}_+ \phi_\sigma\|^2 \leq C (\|V \phi_\sigma\|^2 + \|r^{-1/2} \phi_\sigma\|^2). \quad (4.6)$$

The constant C can be chosen independent of σ in any bounded set.

Proof. Introduce the non-negative symbols

$$\begin{aligned} b_1 &:= 2\kappa^{-1}(X^2 + Y^2) - \chi_+^2, \\ b_2 &:= \kappa^{-1}(X^2 + Y^2) - \chi_+^2, \end{aligned}$$

and let

$$\tilde{B}_1 = 2\kappa^{-1}(\tilde{X}^2 + \tilde{Y}^2) - \tilde{\chi}_+^2.$$

Note that due to (3.8a) and (3.8b)

$$\tilde{B}_1 \equiv 2\kappa^{-1}(\text{Op}^w(X)^2 + \text{Op}^w(Y)^2) - \tilde{\chi}_+^2 \pmod{\Psi(\langle x \rangle^{-1} \langle \xi \rangle^{2q}, g)},$$

and by estimating using the Cauchy-Schwarz inequality

$$\tilde{B}_1 \geq \kappa^{-1}(\text{Op}^w(X)^2 + \text{Op}^w(Y)^2) - \tilde{\chi}_+^2 + R; \quad R \in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{2q}, g).$$

By (3.3)

$$\begin{aligned} \text{Op}^w(X)^2 + \text{Op}^w(Y)^2 - \text{Op}^w(X^2 + Y^2) &\in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{2q}, g), \\ \tilde{\chi}_+^2 - \text{Op}^w(\chi_+^2) &\in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{2q}, g), \end{aligned}$$

so we have proved

$$\tilde{B}_1 \geq \text{Op}^w(b_2) + R; \quad R \in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{2q}, g).$$

With (1.7a) and (3.5) this leads to the bound

$$\tilde{B}_1 \geq -Cr^{-1/2} \langle p \rangle^{2q} r^{-1/2},$$

which in turn due to (4.2) (with $s = -1/2$) leads to

$$\langle \tilde{B}_1 \rangle_{\phi_\sigma} \geq -C (\|r^{-1/2}(\lambda - V)\phi_\sigma\|^2 + \|r^{-1/2}\phi_\sigma\|^2). \quad (4.7)$$

Finally using this bound in combination with (4.5) (with $s = 0$) we conclude that

$$\|\tilde{\chi}_+\phi_\sigma\|^2 \leq C(\|V\phi_\sigma\|^2 + \|r^{-1/2}\phi_\sigma\|^2). \quad (4.8)$$

To complete the proof of (4.6) we need energy bounds. First we note the following quantum version of (1.8),

$$\tilde{\chi}_-^2 + \tilde{\chi}_+^2 = I \pmod{\Psi(\langle x \rangle^{-2}\langle \xi \rangle^{-2}, g)}, \quad (4.9)$$

in particular

$$\tilde{\chi}_+^2 \leq I + R; \quad R \in \Psi(\langle x \rangle^{-2}\langle \xi \rangle^{-2}, g).$$

Whence by commutation

$$\begin{aligned} \tilde{\chi}_+\tilde{X}^2\tilde{\chi}_+ &\leq \tilde{X}\tilde{\chi}_+^2\tilde{X} + C_1r^{-1}\langle p \rangle^{2q}r^{-1} \\ &\leq \tilde{X}^2 + C_2r^{-1}\langle p \rangle^{2q}r^{-1}. \end{aligned} \quad (4.10)$$

Finally, using (4.2) as in (4.7), we estimate

$$\begin{aligned} &\|\langle p \rangle^q\tilde{\chi}_+\phi_\sigma\|^2 \\ &\leq C_1(\|\tilde{X}\tilde{\chi}_+\phi_\sigma\|^2 + \|\tilde{\chi}_+\phi_\sigma\|^2) \quad (\text{by (3.15a)}) \\ &\leq C_1\|\tilde{X}\phi_\sigma\|^2 + C_2(\|r^{-1}\phi_\sigma\|^2 + \|r^{-1}V\phi_\sigma\|^2) + C_1\|\tilde{\chi}_+\phi_\sigma\|^2 \\ &\quad (\text{by (4.10) and (4.2)}) \\ &\leq C(\|V\phi_\sigma\|^2 + \|r^{-1/2}\phi_\sigma\|^2) \quad (\text{by (4.5) and (4.8)}). \end{aligned} \quad (4.11)$$

□

We shall use Lemma 4.1 in conjunction with the following elementary form bound (to treat the last term in the bound). Notice that the operator $\tilde{\chi}_+$ as defined above depends on $\kappa > 0$ and $\sigma \geq 0$.

Lemma 4.2. *Let $s, t \in \mathbb{R}$ with $2s < t \leq 0$ and $\delta > 0$ be given. There exist numbers $n \in \mathbb{N}$ and $C > 0$, possibly depending on $\kappa > 0$ but being independent of $\sigma \geq 0$ in any bounded set, such that with $D := \langle p \rangle^q r^s$*

$$D^*D \leq \delta r^t + C\chi(r \leq n)\langle p \rangle^{2q}\chi(r \leq n) + C\tilde{\chi}_+\langle p \rangle^{2q}\tilde{\chi}_+. \quad (4.12)$$

Proof. Writing $T = D^*D$ and $R_n = \chi(r \leq n)\langle p \rangle^{2q}\chi(r \leq n)$ the calculus and (4.9) lead to (for all large n)

$$\begin{aligned} T &\leq \tilde{\chi}_-T\tilde{\chi}_- + \tilde{\chi}_+T\tilde{\chi}_+ + CD^*r^{-2}D \\ &\leq Cr^{2s}(\chi^2(r \geq n) + \chi^2(r \leq n)) + \tilde{\chi}_+T\tilde{\chi}_+ + CD^*r^{-2}(\chi^2(r \geq n) + \chi^2(r \leq n))D \\ &\leq \frac{\delta}{3}r^t + C\chi(r \leq n)^2r^{2s} + C\tilde{\chi}_+\langle p \rangle^{2q}\tilde{\chi}_+ + D^*(\frac{1}{3} + Cr^{-2}\chi^2(r \leq n))D \\ &\leq \frac{\delta}{3}r^t + CR_n + C\tilde{\chi}_+\langle p \rangle^{2q}\tilde{\chi}_+ + \frac{1}{3}T + CD^*r^{-2}\chi^2(r \leq n)D. \end{aligned}$$

We move the factors of $\chi(r \leq n)$ in the very last term, one to the left and one to the right, yielding the representation of this term

$$\begin{aligned} &C\chi(r \leq n)D^*r^{-2}D\chi(r \leq n) + \text{error} \\ &\leq C_1R_n + D^*\frac{C_2}{n}D. \end{aligned}$$

For the ‘error’ we used the calculus to pick up the bound $O(n^{-1})$. More precisely we used

$$\|[(\chi(r \leq n), D)D^{-1}] + \|(D^*)^{-1}[D^*, (\chi(r \leq n))]\| \leq C/n.$$

Taking n large

$$D^* \frac{C_2}{n} D \leq \frac{1}{3}T,$$

leaving us with the final bound

$$T \leq \frac{\delta}{3}r^t + (C + C_1)R_n + C\tilde{\chi}_+ \langle p \rangle^{2q} \tilde{\chi}_+ + \frac{2}{3}T.$$

This yields (4.12). \square

4.3. Other parameter-dependent bounds. We let $r = r_1$. Rather than considering $e^{\sigma r}$ we now look at e^{f_m} where

$$f_m = f_m(r) = r\sigma + \gamma r/(1 + r/m); m \in \mathbb{N}. \quad (4.13)$$

In Sections 5 and 7 we prove Theorem 1.2 for which the condition $\sigma_c \in (0, \infty)$ is imposed. We shall use this construction for $\sigma \in [0, \sigma_c)$ and small $\gamma \in (0, 1]$. This family of bounded symbols, actually possibly including variation in σ and γ , is uniformly in $S(\langle x \rangle, g)$. Clearly $e^{f_m} \rightarrow e^{(\sigma+\gamma)r}$ for $m \rightarrow \infty$. Since $f_m''(r) = -\frac{2\gamma}{r} \frac{r/m}{(1+r/m)^3} < 0$ we are lacking the convexity property if we replace $e^{\sigma r} \rightarrow e^{f_m}$ in Section 2. So (2.3) is not at our disposal. Note for completeness of discussion that (2.3) could be replaced for example by

$$\begin{aligned} \{X, Y\} &\geq -\frac{2\gamma}{r} ((\partial_\xi X \cdot \omega(x))^2 + (\partial_\xi Y \cdot \omega(x))^2) \\ &\geq -\gamma \frac{C}{r} (X^2 + 1). \end{aligned} \quad (4.14)$$

Here X and Y are defined in terms of f_m (rather than in terms of the exponent σr as before), $\omega(x) = \text{grad } r$, and $C > 0$ is independent of m (and of σ and γ as well). This lack of positivity comes from the second term of (4.13) of course. As we will see in Section 7 a strict positivity near the energy surface coming from the first term of (4.13) can compensate for this deficiency.

In any case as far as energy localization is concerned the rough bound (3.20) suffices. We can proceed as in Subsection 4.2 obtaining the following modification of (4.5), using the similar notation $\phi_m := e^{f_m} \phi$:

$$\|r^s \tilde{Y} \phi_m\|^2 + \|r^s \tilde{X} \phi_m\|^2 \leq 6\|r^s V \phi_m\|^2 + C\|r^{s-1/2} \phi_m\|^2 + C\|V \phi\|^2. \quad (4.15)$$

The constant C can be chosen to be independent of $m \in \mathbb{N}$. We also note that (4.15) is valid under the assumption $r^s e^{f_m} \phi \in L^2$ only, in particular without assuming the strict inequality $\sigma < \sigma_c$. This property with $\sigma = 0$ and $s = 0$, along with a similar modification of Lemma 4.3 below, will be used tacitly in Section 8. Somewhat refined γ -dependent constants can be given, however this will not be relevant for us. The analogue of Lemma 4.1 (based on (4.15) with $s = 0$ and proved similarly) reads:

Lemma 4.3. *For any constants σ and γ as above, for any $\kappa > 0$ and for ϕ_m as above*

$$\|\langle p \rangle^q \tilde{\chi}_+ \phi_m\|^2 \leq C(\|V \phi_m\|^2 + \|r^{-1/2} \phi_m\|^2). \quad (4.16)$$

Here $\chi_+ = \chi(X^2 + Y^2 \geq \kappa)$, and the constant C can be chosen independent of $m \in \mathbb{N}$.

The analogue of Lemma 4.2 (proved similarly) reads:

Lemma 4.4. *Let $s, t \in \mathbb{R}$ with $2s < t \leq 0$ and $\delta > 0$ be given. There exist numbers $n \in \mathbb{N}$ and $C > 0$, possibly depending on σ, γ and κ but being independent of $m \in \mathbb{N}$, such that with $D := \langle p \rangle^q r^s$*

$$D^* D \leq \delta r^t + C \chi(r \leq n) \langle p \rangle^{2q} \chi(r \leq n) + C \tilde{\chi}_+ \langle p \rangle^{2q} \tilde{\chi}_+. \quad (4.17)$$

5. PROOF OF THEOREM 1.2 i)

Suppose (1.3) does not have any solution, i.e. for a small $\kappa > 0$

$$\inf_{\omega, \xi} |Q(\xi + i\sigma_c \omega) - \lambda|^2 \geq 4\kappa > 0.$$

Then we fix $\sigma < \sigma_c$, slightly smaller, and small $\gamma > 0$ with $\sigma + \gamma > \sigma_c$. Define X and Y in terms of the ‘approximation’ f_m considered in Subsection 4.3. We shall show the uniform bound

$$\|\phi_m\|^2 \leq C \|\phi\|^2; \quad \phi_m = e^{f_m} \phi, \quad (5.1)$$

from which we arrive at a contradiction by letting $m \rightarrow \infty$.

Indeed with a proper adjustment of σ and γ we have $X^2 + Y^2 \geq 3\kappa$ for $|x|$ large and for any such $\kappa > 0$ (by an elementary continuity and compactness argument). In particular with the notation of Section 4, $\chi_- = \chi(X^2 + Y^2 \leq \kappa)$ and $\tilde{\chi}_- = \text{Op}^w(\chi_-)$, it follows that $\tilde{\chi}_- \in \Psi(\langle x \rangle^{-2}, g)$. This implies that $\tilde{\chi}_+^2 - I \in \Psi(\langle x \rangle^{-2}, g)$, cf. (4.9). Next by applying Lemma 4.3 we obtain that

$$\begin{aligned} \|\phi_m\|^2 &\leq \|\tilde{\chi}_+ \phi_m\|^2 + C_1 \|r^{-1} \phi_m\|^2 \\ &\leq C (\|V \phi_m\|^2 + \|r^{-1/2} \phi_m\|^2). \end{aligned} \quad (5.2)$$

Clearly (5.1) follows from (5.2).

6. PROOF OF THEOREM 1.3

Let $r = r_\epsilon$ for $\epsilon \in (0, 1)$ and let $\omega = \omega(x) = \text{grad } r$. Using Sections 3 and 4 we shall give the missing details in the outline of proof of Theorem 1.3 given in Section 2. So suppose that the equations (1.4) do not have solutions. We look at the state $\phi_\sigma = e^{\sigma r} \phi$, with $\sigma < \sigma_c$ but close, and want to prove (2.7).

We introduce

$$\hat{S}_{\sigma, \lambda} = \{(x, \xi) \in (\mathbb{R}^d \setminus \{0\}) \times \mathbb{R}^d \mid Q(\xi + i\sigma \hat{x}) = \lambda\}, \quad (6.1)$$

which at infinity (i.e. for $|x|$ large) is close to the set $S_{\sigma, \lambda}$ of (2.1). We localize near $\hat{S}_{\sigma, \lambda}$ introducing the quantization $\tilde{\chi}_-$ of the symbol $\chi_- = \chi(X^2 + Y^2 \leq \kappa)$, $\kappa > 0$ small. This notation conforms with the notation of Section 2 and Subsection 4.2 (in particular as in Subsection 4.2 the dependence on κ is suppressed).

Now we implement the ideas of Section 2. There is a small complication from quantization that is not discussed there (making in fact (2.5) slightly misleading). This relates to (3.8b). The following formula (which for example is deducible from (3.1)) is obviously an improvement

$$\begin{aligned} \tilde{Y} - \text{Op}^w(Y) - R &\in \Psi(\langle x \rangle^{-2} \langle \xi \rangle^{q-2}, g); \\ R &= \frac{1}{2} \text{Op}^w(\nabla_x \cdot \nabla_\xi X) \in \Psi(\langle x \rangle^{-1} \langle \xi \rangle^{q-2}, g). \end{aligned} \quad (6.2)$$

However we are not going to use (6.2). The formula serves as some motivation for the following argument for a lower bound of the quantity $2\text{Re}(A_c\tilde{Y})$, where as in Section 2 our conjugate operator is $A_c = \text{Op}^w(rY)$. We write (3.8b) on the form

$$\tilde{Y} = \text{Op}^w(Y) + R_{-1} \text{ where } R_{-1} \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^q, g),$$

and note, cf. (3.3), that

$$A_c = \text{Op}^w(Y)r + \frac{i}{2}\text{Op}^w(\{Y, r\}) \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^q, g).$$

The second term to the right is anti-symmetric and whence (using (3.3) again)

$$\text{Re}\left(\frac{i}{2}\text{Op}^w(\{Y, r\})\tilde{Y}\right) \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^{2q}, g).$$

These facts lead to

$$\text{Re}(A_c\tilde{Y}) - \tilde{Y}r\tilde{Y} + \text{Re}(R_{-1}r\tilde{Y}) \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^{2q}, g).$$

Using the Cauchy-Schwarz inequality this leads for example to

$$2\text{Re}(A_c\tilde{Y}) \geq \frac{3}{2}\tilde{Y}r\tilde{Y} + R; \quad R \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^{2q}, g). \quad (6.3)$$

Using (6.3) and arguing similarly we get the estimate

$$B_1 := 2\text{Re}(A_c\tilde{Y}) + \text{Op}^w(\{X, r\}Y) \geq \tilde{Y}r\tilde{Y} + R; \quad R \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^{2q}, g). \quad (6.4)$$

Letting

$$b_2 = r\{X, Y\} \text{ and } B_2 = \text{Op}^w(b_2) \in \Psi(\langle \xi \rangle^{2q}, g)$$

we calculate using (3.8a)

$$2\text{Im}(A_c(\tilde{X} + i\tilde{Y})) - B_1 - B_2 \in \Psi(\langle x \rangle^{-1}\langle \xi \rangle^{2q}, g). \quad (6.5)$$

We obtain from (1.7a), (6.4) and (6.5) that

$$2\text{Im}(A_c(\tilde{X} + i\tilde{Y})) \geq B_2 + \tilde{Y}r\tilde{Y} - Cr^{-1/2}\langle p \rangle^{2q}r^{-1/2}. \quad (6.6)$$

Next we use (2.2) and our assumption that the equations (1.4) do not have solutions (and a continuity and compactness argument) to obtain: There exists $c > 0$ such that for all small κ and for all large $|x|$

$$(b_2 - 3cr^{-\epsilon})\chi_-^2 \geq 0. \quad (6.7)$$

In combination with (3.5) and (6.6) we thus get that for all small κ

$$\begin{aligned} 2\text{Im}(A_c(\tilde{X} + i\tilde{Y})) &\geq 2cr^{-\epsilon} + \tilde{Y}r\tilde{Y} - C_1\tilde{\chi}_+\langle p \rangle^{2q}\tilde{\chi}_+ + B; \\ B &= cr^{-\epsilon} - C_2r^{-1/2}\langle p \rangle^{2q}r^{-1/2}. \end{aligned} \quad (6.8)$$

Next we invoke Lemma 4.2 (with $s = -1/2$, $t = -\epsilon$ and $\delta = c/C_2$) and conclude that for some small κ and some large n

$$\begin{aligned} 2\text{Im}(A_c(\tilde{X} + i\tilde{Y})) \\ \geq 2cr^{-\epsilon} + \tilde{Y}r\tilde{Y} - C\tilde{\chi}_+\langle p \rangle^{2q}\tilde{\chi}_+ - C\chi(r \leq n)\langle p \rangle^{2q}\chi(r \leq n). \end{aligned} \quad (6.9)$$

We apply this form identity to ϕ_σ noting here (and henceforth) the interpretation

$$\langle 2\text{Im}(A_c(\tilde{X} + i\tilde{Y})) \rangle_{\phi_\sigma} = 2\text{Im}\langle A_c\phi_\sigma, (\tilde{X} + i\tilde{Y})\phi_\sigma \rangle.$$

With Lemma 4.1 this leads to

$$2c\|r^{-\epsilon/2}\phi_\sigma\|^2 \leq -\langle i[V, A_c] \rangle_{\phi_\sigma} - \|r^{1/2}\tilde{Y}\phi_\sigma\|^2 + C_1\|V\phi_\sigma\|^2 + C_2\|r^{-1/2}\phi_\sigma\|^2 + C_3\|\phi\|_{H^a}^2.$$

Since V is bounded the H^q -norm appearing to the right can be replaced by the L^2 -norm due to (3.10) with $f = 0$ and $\psi = \phi$. Whence using that $V = O(|x|^{-\delta})$, $\delta = \min(\delta_1, \delta_2)$, we obtain the bound (2.6) for $\epsilon < \min(2\delta_1, 2\delta_2, 1)$, that is

$$c\|r^{-\epsilon/2}\phi_\sigma\|^2 \leq -\langle i[V, A_c] \rangle_{\phi_\sigma} - \|r^{1/2}\tilde{Y}\phi_\sigma\|^2 + C\|\phi\|^2. \quad (6.10)$$

Using the conditions on V_1 and V_2 and (6.10), assuming also $\epsilon < \min(\delta_1, 2\delta_2)$, and (3.15a) and (4.5) we can show (2.7) as follows: We estimate

$$-\langle i[V_1, A_c] \rangle_{\phi_\sigma} \leq C_1\|\langle p \rangle^q r^{-\delta_1/2}\phi_\sigma\|^2 \leq C_2\|r^{-\delta_1/2}\phi_\sigma\|^2, \quad (6.11a)$$

$$-\langle i[V_2, A_c] \rangle_{\phi_\sigma} \leq C_1\|r^{-\delta_2}\phi_\sigma\|^2 + \|r^{1/2}\tilde{Y}\phi_\sigma\|^2 + C_2\|r^{-1/2}\phi_\sigma\|^2, \quad (6.11b)$$

and insert into (6.10) leading to the uniform bound

$$\frac{c}{2}\|r^{-\epsilon/2}\phi_\sigma\|^2 \leq C\|\phi\|^2.$$

Now take $\sigma \nearrow \sigma_c$.

7. PROOF OF THEOREM 1.2 ii)

Let $r = r_1$, and let $\omega(x) = \text{grad } r$. Note that $\omega'(x) = r^{-1}P_\perp(\omega(x))$. We suppose that the conditions (1.2a) and (1.2b) are not both true at any point (ω, ξ) and want to find a contradiction. For that we look at the state $\phi_\sigma = e^{\sigma r}\phi$ where $\sigma < \sigma_c$, but close. As a first step (serving mainly as a warm up) we are heading towards the following analogue of (2.7) which we will show to be uniform in $\sigma < \sigma_c$:

$$\|\phi_\sigma\|^2 \leq C\|\phi\|^2. \quad (7.1)$$

Let $\hat{S}_{\sigma, \lambda}$ be defined by (6.1). Note that (6.6) is at our disposal. By continuity and compactness we have uniformly in σ close to σ_c ,

$$\begin{aligned} & \nabla_\xi X(\xi + i\sigma\hat{x})P_\perp(\hat{x})\nabla_\xi X(\xi + i\sigma\hat{x}) \\ & + \nabla_\eta X(\xi + i\sigma\hat{x})P_\perp(\hat{x})\nabla_\eta X(\xi + i\sigma\hat{x}) \geq \check{c} > 0 \end{aligned} \quad (7.2)$$

for all points in $(x, \xi) \in \hat{S}_{\sigma, \lambda}$.

Note this is valid for $\sigma = \sigma_c$ in a neighbourhood of $\hat{S}_{\sigma_c, \lambda}$. We can freely replace \hat{x} by $\omega(x)$ in (7.2) (since only large $|x|$ matters below), and this slight extension of (7.2) leads to the following analogue of (6.7) (with $b_2 = r\{X, Y\}$ as before),

$$(b_2 - 3c)\chi_-^2 \geq 0. \quad (7.3)$$

As in (6.7) this is for all small κ and for all large $|x|$. From here we continue mimicking Section 6 and come to the following analogue of (6.10) (using now only that $V = o(|x|^0)$),

$$c\|\phi_\sigma\|^2 \leq -\langle i[V, A] \rangle_{\phi_\sigma} - \|r^{1/2}\tilde{Y}\phi_\sigma\|^2 + C\|\phi\|^2.$$

Next by using this and minor modifications of (6.11a) and (6.11b) we indeed obtain (7.1). By taking $\sigma \nearrow \sigma_c$ we conclude that $e^{\sigma|x|}\phi \in L^2$ with $\sigma = \sigma_c$.

The next step is to use Subsection 4.3 to show that $e^{\sigma|x|}\phi \in L^2$ with σ slightly bigger, which obviously is a contradiction. We mimic Section 5. So fix $\sigma < \sigma_c$, slightly smaller, and small $\gamma > 0$ with $\sigma + \gamma > \sigma_c$. Define X and Y in terms of the approximation f_m considered in Subsection 4.3 and consider the corresponding

state $\phi_m = e^{f_m}\phi$. Using Lemmas 4.3 and 4.4 (rather than Lemmas 4.1 and 4.2) mimicking Section 6 we obtain (as above) the following version of (6.10),

$$c\|\phi_m\|^2 \leq -\langle i[V, A] \rangle_{\phi_m} - \|r^{1/2}\tilde{Y}\phi_m\|^2 + C\|\phi\|^2.$$

Notice at this point that the lack of positivity encountered in (4.14) is resolved using (7.2) and the smallness of γ , cf. (8.2) below. Estimating the commutator (as above) we arrive at the estimate

$$\|\phi_m\|^2 \leq C\|\phi\|^2.$$

We obtain a contradiction by letting $m \rightarrow \infty$.

8. PROOF OF THEOREM 1.1

If $\lambda \notin \text{Ran}Q$ and $V(x) = o(1)$ at infinity (so that V is a relatively compact perturbation of $Q(p)$) we can use the Combes-Thomas method [CT] to see that indeed $\sigma_c > 0$. We omit the details.

As for proving $\sigma_c > 0$ under the condition 2) of Theorem 1.1 we take $\sigma = 0$ and $r = r_1$ in (4.13). Whence we consider

$$f_m := \gamma r(1 + r/m)^{-1}; \quad \gamma \in (0, 1] \text{ and } m \in \mathbb{N}.$$

Abbreviating $\phi_m = e^{f_m}\phi$ we shall for a sufficiently small γ prove the estimate

$$\|\phi_m\|^2 \leq C\|\phi\|^2. \quad (8.1)$$

Taking $m \rightarrow \infty$ in (8.1) yields $e^{\gamma r}\phi \in L^2$ completing the proof of Theorem 1.1.

An elementary computation shows

$$\nabla f_m(x) = \gamma g_m(r)\omega(x); \quad g_m := (1 + r/m)^{-2}, \quad \omega = \nabla r. \quad (8.2)$$

In agreement with the previous sections we consider the operators \tilde{X} and \tilde{Y} with approximate symbols X_m and Y_m , respectively, given by conjugation by e^{f_m} (here and below we partly use the subscript m to stress the dependence on this parameter). We are going to construct a conjugate operator. The previous sections suggest the quantization of rY_m , however we prefer to use this symbol with a different normalization: Rather we consider

$$a_c(x, \xi) = r/(\gamma g_m(r))Y_m(x, \xi) \text{ and } A_c = \text{Op}^w(a_c).$$

It follows from (3.7) that $a_c \in S(r\langle \xi \rangle^q, g)$ uniformly in m , in fact by (3.7)

$$Y_m/(\gamma g_m(r)) = \nabla Q(\xi) \cdot \omega + \gamma y_{0,\gamma,m} = \tilde{y}_{0,\gamma,m}, \quad (8.3)$$

where $y_{0,\gamma,m}, \tilde{y}_{0,\gamma,m} \in S(\langle \xi \rangle^q, g)$ uniformly in γ and m . We define $\tilde{Y}_{0,\gamma,m} = \text{Op}^w(\tilde{y}_{0,\gamma,m})$ allowing us to write, cf. (3.8b),

$$\begin{aligned} \tilde{Y} &= \gamma g_m(r)(\tilde{Y}_{0,\gamma,m} + \text{Op}^w(\tilde{y}_{-1,\gamma,m})), \\ A_c &= \text{Op}^w(r\tilde{y}_{0,\gamma,m}) = \tilde{Y}_{0,\gamma,m}r + \text{Op}^w(y_{0,\gamma,m}^c), \end{aligned}$$

where $y_{0,\gamma,m}^c \in S(\langle \xi \rangle^q, g)$ and $\tilde{y}_{-1,\gamma,m} \in S(r^{-1}\langle \xi \rangle^q, g)$, both uniformly in γ and m . This yields

$$\begin{aligned} \gamma^{-1}\text{Re}(A_c\tilde{Y}) &= \tilde{Y}_{0,\gamma,m}g_m(r)r\tilde{Y}_{0,\gamma,m} + \text{Re}(\text{Op}^w(y_{0,\gamma,m}^c)g_m(r)\text{Op}^w(\tilde{y}_{-1,\gamma,m})) \\ &\quad + \text{Re}(\tilde{Y}_{0,\gamma,m}r\text{Op}^w(\tilde{y}_{-1,\gamma,m})) + \text{Re}(\text{Op}^w(y_{0,\gamma,m}^c)g_m(r)\tilde{Y}_{0,\gamma,m}). \end{aligned}$$

The first term to the right is non-negative, and for the other terms we can use (1.7a) leading to

$$\operatorname{Re}(A_c \tilde{Y}) \geq -C\gamma \langle p \rangle^{2q}, \text{ uniformly in } m. \quad (8.4)$$

Next by (3.7) and (8.3)

$$\{X_m, a_c\} = \{X_m, r\check{y}_{0,\gamma,m}\} = |\nabla Q(\xi)|^2 + \gamma a_{0,\gamma,m},$$

where $a_{0,\gamma,m} \in S(\langle \xi \rangle^{2q}, g)$ uniformly in γ and m .

Whence, cf. (3.8a),

$$2\operatorname{Im}(A_c \tilde{X}) \geq |\nabla Q(p)|^2 - C\gamma \langle p \rangle^{2q} - Cr^{-1/2} \langle p \rangle^{2q} r^{-1/2}. \quad (8.5)$$

Introducing functions $\chi_{-,m} = \chi(X_m^2 + Y_m^2 \leq \kappa)$ and $\chi_{+,m} = \chi(X_m^2 + Y_m^2 \geq \kappa)$ we have for small $\kappa, \gamma > 0$ and for large $|x|$

$$(|\nabla Q(\xi)|^2 - 3c)\chi_{-,m}^2 \geq 0, \quad (8.6)$$

cf. (6.7). Note that due to the condition 2) of Theorem 1.1 such $c > 0$ exists and it can be chosen to be independent of m . Combining this with (8.4) and (8.5) gives the following analogue of (6.8)

$$\begin{aligned} 2\operatorname{Im}(A_c(\tilde{X} + i\tilde{Y})) &\geq 2c - C_1 \tilde{\chi}_{+,m} \langle p \rangle^{2q} \tilde{\chi}_{+,m} + B; \\ B &= c - C_2\gamma - C_3 r^{-1/2} \langle p \rangle^{2q} r^{-1/2}. \end{aligned}$$

At this point we fix a small γ such that $\delta := (c - C_2\gamma)/C_3 > 0$. As before, now using Lemma 4.4 with this δ , it follows that for some large n

$$2\operatorname{Im}(A_c(\tilde{X} + i\tilde{Y})) \geq 2c - C \tilde{\chi}_{+,m} \langle p \rangle^{2q} \tilde{\chi}_{+,m} - C\chi(r \leq n) \langle p \rangle^{2q} \chi(r \leq n),$$

where C is independent of m . We apply this estimate to the state $\phi_{m,k} := \chi(r \leq k)\phi_m$. Taking $k \rightarrow \infty$ by using Lebesgue's dominated convergence theorem leaves us, in conjunction with Lemma 4.3, with

$$2c\|\phi_m\|^2 \leq -\langle i[V, A_c] \rangle_{\phi_m} + C_1\|V\phi_m\|^2 + C_2\|r^{-1/2}\phi_m\|^2 + C_3\|\phi\|_{H^q}^2.$$

Since $V = o(r^0)$ we then obtain

$$c\|\phi_m\|^2 \leq -\langle i[V, A_c] \rangle_{\phi_m} + C\|\phi\|^2. \quad (8.7)$$

By using the conditions on V_1 and V_2 and the partition $\chi(r \leq n)^2 + \chi(r > n)^2 = I$ (for n large) combined with for example (3.15a) and (4.15) (with $t = s = 0$) we can estimate

$$-\langle i[V_1, A_c] \rangle_{\phi_m} \leq \frac{\epsilon}{4}\|\phi_m\|^2 + C\|\phi\|^2, \quad (8.8a)$$

$$-\langle i[V_2, A_c] \rangle_{\phi_m} = -2\operatorname{Im} \langle r^{-1}A_c\phi_m, rV_2\phi_m \rangle \leq \frac{\epsilon}{4}\|\phi_m\|^2 + C\|\phi\|^2. \quad (8.8b)$$

We insert (8.8a) and (8.8b) into (8.7) leading to the uniform bound

$$\frac{\epsilon}{2}\|\phi_m\|^2 \leq C\|\phi\|^2,$$

and therefore (8.1).

9. PROOF OF THEOREMS 1.4 AND 1.5

Let $r = r_\epsilon$, and let $\omega = \omega(x) = \text{grad } r$. Defining

$$a = (a_1, \dots, a_d) = e^{-\sigma r} p e^{\sigma r} = p - i\sigma\omega, \quad (9.1)$$

consider

$$e^{-\sigma r} Q(p) e^{\sigma r} = Q(p - i\sigma\omega) = Q(a).$$

For the proof of Theorem 1.4 positivity properties of $[Q(a^*), Q(a)]$ will be crucial. We shall completely abandon the use of the pseudodifferential calculus, in particular we shall not use the symbols X and Y . Rather we are going to do exact calculations of the above commutator. Note that $p_{kl} := [a_k, a_l^*] = 2\sigma\partial_l\omega_k$, and thus $P := (p_{kl}) = 2\sigma\omega' \geq c\sigma r^{-1-\epsilon} > 0$.

From (2.2) (or for other reasons) one might guess that to “leading order”

$$[Q(a), Q(a^*)] \approx 2\sigma Q'(a)\omega'Q'(a^*)^T \geq 0. \quad (9.2)$$

However this analogy with the previous sections turns out to be somewhat misleading, or at least insufficient, for the problem at hand. From the viewpoint of the calculus of pseudodifferential operators there is a competition in a symbol between the behaviour as the phase-space variables $\rightarrow \infty$ and the behaviour when $\sigma \rightarrow \infty$ and it is natural to use a suitable parameter-dependent calculus, see Subsubsection 9.4.1 for a possible candidate. But even with such a device this competition appears too subtle to be resolved (at least for us) and consequently we are going to do *exact* calculations on the commutator $[Q(a), Q(a^*)]$. Those belong to the functional calculus rather than the pseudodifferential calculus. We shall derive a combinatorial formula in which the “total amount” of positivity in $[Q(a), Q(a^*)]$ is explicitly exposed. The expression in (9.2) turns out to be only one out of in general many positive expressions “hidden” in the commutator. The other expressions would in the framework of the previous sections be considered as harmless lower order terms. In the present context they also have “lower order”. Nevertheless as the reader will see we will need all of them.

9.1. Calculation of a commutator. For each $m \geq 1$, let $J_m = (j_1, \dots, j_m)$ and $K_m = (k_1, \dots, k_m)$ be m -tuples of numbers in $\{1, \dots, d\}$. In this section we will prove the following formula:

$$[Q(a), Q(a^*)] = F + E; \quad (9.3)$$

$$F = \sum_{m \geq 1, J_m, K_m} (m!)^{-1} (\partial_{j_1} \cdots \partial_{j_m} Q)(a^*) \left(\prod_{l=1}^m p_{j_l k_l} \right) (\partial_{k_1} \cdots \partial_{k_m} Q)(a),$$

$$E = \sum_{m \geq 1, J_m, K_m, \bar{\alpha} + \bar{\beta} \neq 0} c_{J_m, K_m}^{\bar{\alpha}, \bar{\beta}} (\partial^\alpha \partial_{j_1} \cdots \partial_{j_m} Q)(a^*) P_{J_m, K_m}^{\bar{\alpha}, \bar{\beta}} (\partial^\beta \partial_{k_1} \cdots \partial_{k_m} Q)(a),$$

where the summation parameters $\bar{\alpha} = (\alpha_1, \dots, \alpha_m)$ and $\bar{\beta} = (\beta_1, \dots, \beta_m)$ for the sum E denote arbitrary m -tuples of multi-indices, $\alpha = \sum_{l=1}^m \alpha_l$, $\beta = \sum_{l=1}^m \beta_l$, and $P_{J_m, K_m}^{\bar{\alpha}, \bar{\beta}} = (\partial^{\alpha_1 + \beta_1} p_{j_1 k_1}) \cdots (\partial^{\alpha_m + \beta_m} p_{j_m k_m})$. We will not need an explicit expression

for the combinatorial coefficient $c_{J_m, K_m}^{\bar{\alpha}, \bar{\beta}}$ because for σ large, the term E will be seen to be negligible.

To prove (9.3) let $\text{ad}_b(c) = [b, c]$, $r_b(c) = cb$, $l_b(c) = bc$. Note that for commuting b_1 and b_2 all the operators ad_{b_1} , ad_{b_2} , r_{b_1} , r_{b_2} , l_{b_1} , l_{b_2} commute. For f a polynomial in d variables and b_1, b_2, \dots, b_d commuting operators, we note the Taylor type formulas

$$\begin{aligned} [f(b), c] &= (f(\text{ad}_b + r_b) - f(r_b))c \\ &= \sum_{\alpha \neq 0} (\alpha!)^{-1} \text{ad}_b^\alpha(c) \partial^\alpha f(b), \end{aligned} \quad (9.4a)$$

$$\begin{aligned} [f(b), c] &= (f(l_b) - f(-\text{ad}_b + l_b))c \\ &= \sum_{\alpha \neq 0} \frac{(-1)^{|\alpha|+1}}{\alpha!} \partial^\alpha f(b) \text{ad}_b^\alpha(c). \end{aligned} \quad (9.4b)$$

We will also need the Leibniz type formula

$$\text{ad}_b^\alpha(cd) = \sum_{\gamma} \binom{\alpha}{\gamma} \text{ad}_b^{\alpha-\gamma}(c) \text{ad}_b^\gamma(d). \quad (9.5)$$

By (9.4a) and (9.4b)

$$[Q(a), Q(a^*)] = \sum_{\alpha \neq 0} (\alpha!)^{-1} (\text{ad}_a^\alpha Q(a^*)) Q^{(\alpha)}(a), \quad (9.6)$$

$$[a_j, Q(a^*)] = \sum_{\alpha \neq 0} \frac{(-1)^\alpha}{\alpha!} Q^{(\alpha)}(a^*) \text{ad}_{a^*}^\alpha a_j. \quad (9.7)$$

Here and below we denote $g^{(\alpha)} = \partial^\alpha g$, $(-1)^\alpha = (-1)^{|\alpha|}$ and $\text{ad}_b^\alpha c = \text{ad}_b^\alpha(c)$.

We will use the summation rule

$$\sum_{\alpha \neq 0} f(\alpha) = \sum_{\beta, k} \zeta(\beta + e_k) f(\beta + e_k), \quad (9.8)$$

where for $\alpha \neq 0$, $\zeta(\alpha)^{-1} =$ the number of j 's with $\alpha_j > 0$, and $\{e_1, \dots, e_d\}$ is the standard basis for \mathbb{R}^d . Note that the number of pairs (β, k) such that $\alpha = \beta + e_k$ is the number of j 's such that $\alpha_j > 0$.

Introducing also the notation $d(\alpha) = (\alpha!)^{-1} \zeta(\alpha)$ it follows that

$$\text{ad}_a^{\alpha+e_j} Q(a^*) = \sum_{\beta, \gamma, \mu, k, \gamma+\mu=\alpha} \frac{\text{ad}_a^\mu Q^{(\beta+e_k)}(a^*)}{\mu!} \left\{ (-1)^\beta d(\beta + e_k) \frac{\alpha!}{\gamma!} \text{ad}_a^{\beta+\gamma} p_{jk} \right\}. \quad (9.9)$$

Here we used (9.5), (9.7), (9.8), the computation $\text{ad}_{a^*}^\alpha a_j = -p_{jk}$ and whence that

$$\text{ad}_a^\gamma \text{ad}_{a^*}^{\beta+e_k} a_j = -\text{ad}_a^{\gamma+\beta} p_{jk} = -\text{ad}_a^{\beta+\gamma} p_{jk}.$$

Thus for $f(\mu) = Q^{(\mu)}(a)$ (or any other operator-valued function f) and with

$$\lambda(\beta, \gamma, \mu, j, k) := \frac{(\gamma+\mu)!}{\gamma!} d(\beta + e_k) d(\gamma + \mu + e_j),$$

$$\begin{aligned} & \sum_{\mu \neq 0} \frac{\text{ad}_a^\mu Q(a^*)}{\mu!} f(\mu) \\ &= \sum_{\beta, \gamma, j, k, \mu} \frac{\text{ad}_a^\mu Q^{(\beta+e_k)}(a^*)}{\mu!} \left\{ (-1)^\beta \lambda(\beta, \gamma, \mu, j, k) \text{ad}_a^{\beta+\gamma} (p_{jk}) f(\gamma + \mu + e_j) \right\} \\ &= \sum_{\beta, \gamma, j, k} Q^{(\beta+e_k)}(a^*) \left\{ (-1)^\beta d(\beta + e_k) d(\gamma + e_j) \text{ad}_a^{\beta+\gamma} (p_{jk}) f(\gamma + e_j) \right\} \\ & \quad + \sum_{\beta, \gamma, j, k} \sum_{\mu \neq 0} \frac{\text{ad}_a^\mu Q^{(\beta+e_k)}(a^*)}{\mu!} \left\{ (-1)^\beta \lambda(\beta, \gamma, \mu, j, k) \text{ad}_a^{\beta+\gamma} (p_{jk}) f(\gamma + e_j + \mu) \right\}. \end{aligned} \quad (9.10)$$

Here we have used (9.8) and (9.9).

From (9.10) we can proceed inductively. Introduce the notation

$$\begin{aligned} B_l &= (\beta_1, \dots, \beta_l), & \Gamma_l &= (\gamma_1, \dots, \gamma_l), \\ J_l &= (j_1, \dots, j_l), & K_l &= (k_1, \dots, k_l), \\ p_{jk\beta\gamma} &= \partial^{\beta+\gamma} p_{jk}, & D &= -i\partial. \end{aligned}$$

Here the components of B_l and Γ_l are multi-indices, while the components of J_l and K_l are numbers in $\{1, \dots, d\}$.

Repeatedly using (9.10) we obtain

$$\begin{aligned} [Q(a), Q(a^*)] &= \sum_{\beta, \gamma, j, k} d(\beta + e_k) d(\gamma + e_j) (D^{\beta+e_k} Q)(a)^* p_{jk\beta\gamma} (D^{\gamma+e_j} Q)(a) \quad (9.11) \\ &+ \sum_{m \geq 2, B_m, \Gamma_m, J_m, K_m} C_{J_m, K_m}^{B_m, \Gamma_m} (D^{\sum_{l=1}^m (\beta_l + e_{k_l})} Q)(a)^* \left(\prod_{l=1}^m p_{j_l k_l \beta_l \gamma_l} \right) (D^{\sum_{l=1}^m (\gamma_l + e_{j_l})} Q)(a). \end{aligned}$$

Here

$$C_{J_m, K_m}^{B_m, \Gamma_m} = \left(\prod_{l=1}^m \frac{d(\beta_l + e_{k_l})}{\gamma_l!} \right) \prod_{l=1}^m \left((\gamma_l + \sum_{k=l+1}^m (\gamma_k + e_{j_k}))! d(\sum_{k=l}^m (\gamma_k + e_{j_k})) \right),$$

where the empty sum, $\sum_{k=m+1}^m$, is by convention $= 0$. Note that if $\beta_j = \gamma_j = 0$ for all j then we have

$$C_{J_m, K_m}^{B_m, \Gamma_m} = C_{J_m} := \left((\sum_{k=1}^m e_{j_k})! \right)^{-1} \prod_{l=1}^m \zeta(\sum_{k=l}^m e_{j_k}).$$

To compute the first term in (9.3) note that in (9.11) we can replace C_{J_m} by its average over permutations. To compute this we use (9.8) and compute as a formal sum

$$\begin{aligned} \Sigma_\alpha f(\alpha) &= f(0) + \Sigma_{\alpha, j} f(\alpha + e_j) \zeta(\alpha + e_j) \\ &= f(0) + \Sigma_j f(e_j) \zeta(e_j) + \sum_{\alpha, j_1, j_2} f(\alpha + e_{j_1} + e_{j_2}) \zeta(\alpha + e_{j_1} + e_{j_2}) \zeta(\alpha + e_{j_2}) \\ &= f(0) + \sum_{m \geq 1, J_m} \left(f(\sum_{l=1}^m e_{j_l}) \prod_{k=1}^m \zeta(\sum_{l=k}^m e_{j_l}) \right). \end{aligned}$$

We set $f(\alpha) = x^\alpha / \alpha!$ and obtain

$$\begin{aligned} e^{(x_1 + x_2 + \dots + x_d)} &= 1 + \sum_{m \geq 1, J_m} \frac{x^{(e_{j_1} + e_{j_2} + \dots + e_{j_m})}}{(e_{j_1} + e_{j_2} + \dots + e_{j_m})!} \prod_{k=1}^m \zeta(\sum_{l=k}^m e_{j_l}) \\ &= 1 + \sum_{m \geq 1, J_m} C_{J_m} x^{(e_{j_1} + e_{j_2} + \dots + e_{j_m})}. \end{aligned}$$

Differentiating and then setting $x = 0$ gives

$$1 = \frac{\partial^m e^{(x_1 + x_2 + \dots + x_d)}}{\partial x_{k_1} \dots \partial x_{k_m}} \Big|_{x=0} = \sum_{\sigma \in \mathcal{S}_m} C_{k_{\sigma(1)}, \dots, k_{\sigma(m)}}.$$

It follows that

$$F = \sum_{m \geq 1} (m!)^{-1} \sum_{J_m, K_m} (D^{\sum_{l=1}^m e_{k_l}} Q)(a)^* \left(\prod_{l=1}^m p_{j_l k_l} \right) (D^{\sum_{l=1}^m e_{j_l}} Q)(a),$$

which is (9.3) with E given with reference to (9.11).

9.2. **Proof of Theorem 1.4.** The positivity of F comes from the inequality

$$P \otimes \cdots \otimes P \geq c\sigma^m r^{-(1+\epsilon)m} I \quad (9.12)$$

on $\otimes_{j=1}^m l^2(\{1, \dots, d\})$ for some $c > 0$. This gives

$$CF \geq \sum_{\alpha \neq 0} \sigma^{|\alpha|} \partial^\alpha Q(a^*) r^{-(1+\epsilon)|\alpha|} \partial^\alpha Q(a). \quad (9.13)$$

A typical term in E can be written

$$T = \sigma^m \partial^{\alpha+\mu} Q(a^*) R_{\alpha,\beta,\mu,\nu} \partial^{\beta+\nu} Q(a),$$

where $|\alpha| = |\beta| = m$, $\mu + \nu \neq 0$, and $|R_{\alpha,\beta,\mu,\nu}| \leq Cr^{-m-|\mu|-|\nu|}$. It follows that

$$\begin{aligned} \pm \operatorname{Re}(T) &\leq C(\sigma^m \lambda \partial^{\alpha+\mu} Q(a^*) r^{-m-|\mu|-|\nu|} \partial^{\alpha+\mu} Q(a) \\ &\quad + \sigma^m \lambda^{-1} \partial^{\beta+\nu} Q(a^*) r^{-m-|\mu|-|\nu|} \partial^{\beta+\nu} Q(a)). \end{aligned}$$

If one of the multi-indices μ or ν is zero, say $\nu = 0$, then take $\lambda = \sigma^{1/2}$. Otherwise take $\lambda = 1$. If we take $\epsilon < 1/q$ clearly this term is negligible compared to F for large σ . It follows that E is negligible compared to F for large σ .

Let us now prove Theorem 1.4. We have $(Q(a^*) + V_1 - \lambda)\phi_\sigma = -V_2\phi_\sigma$ which gives

$$\begin{aligned} (\phi_\sigma, [Q(a), Q(a^*)]\phi_\sigma) + 2\operatorname{Re}(\phi_\sigma, [Q(a), V_1]\phi_\sigma) + \|(Q(a) + V_1 - \lambda)\phi_\sigma\|^2 \\ = \|V_2\phi_\sigma\|^2. \end{aligned} \quad (9.14)$$

We use (9.4a) to compute $[Q(a), V_1]$:

$$\begin{aligned} [Q(a), V_1] &= \sum_{\alpha \neq 0} (\alpha!)^{-1} (\operatorname{ad}_a^\alpha V_1) \partial^\alpha Q(a) \\ &= \sum_{\alpha \neq 0} (\alpha!)^{-1} ((-i\partial)^\alpha V_1) \partial^\alpha Q(a). \end{aligned} \quad (9.15)$$

With the Cauchy-Schwarz inequality we can bound

$$-2\operatorname{Re}(\phi_\sigma, [Q(a), V_1]\phi_\sigma) \leq C \sum_{1 \leq |\alpha| \leq q} (r^{(1+\epsilon)|\alpha|} (\partial^\alpha V_1)^2 + \partial^\alpha Q(a^*) r^{-(1+\epsilon)|\alpha|} \partial^\alpha Q(a)).$$

The fact that $\phi_\sigma = 0$ follows by taking ϵ small and then using the formula (9.13). In addition the terms with $m = q$ in (9.13) are used to bound $|V_2|^2$ and the terms $r^{(1+\epsilon)|\alpha|} (\partial^\alpha V_1)^2$. This completes the proof of Theorem 1.4.

In the next subsection we display additional positivity of $[Q(a), Q(a^*)]$ by giving a symmetrized estimate. This will be important in proving Theorem 1.5.

9.3. **Symmetrized estimate.** Abbreviating $r^{-(1+\epsilon)|\alpha|} = R_\alpha$, $\partial^\alpha Q = Q^{(\alpha)}$ we will show here that for some $C > 0$ and all large σ

$$C[Q(a), Q(a^*)] \geq \sum_{\alpha \neq 0} \sigma^{|\alpha|} (Q^{(\alpha)}(a^*) R_\alpha Q^{(\alpha)}(a) + Q^{(\alpha)}(a) R_\alpha Q^{(\alpha)}(a^*)). \quad (9.16)$$

For any $m \geq 1$ we abbreviate $J = (j_1, \dots, j_m)$, $K = (k_1, \dots, k_m)$, $\partial_J = \partial_{j_1} \cdots \partial_{j_m}$, $P_{JK} = p_{j_1 k_1} \cdots p_{j_m k_m}$. We introduce

$$\begin{aligned} F_{\text{left}} &= \sum_{m, J, K} (m!)^{-1} \partial_J Q(a^*) P_{JK} \partial_K Q(a), \\ F_{\text{right}} &= \sum_{m, J, K} (m!)^{-1} \partial_K Q(a) P_{KJ} \partial_J Q(a^*). \end{aligned}$$

Clearly $F = F_{\text{left}}$, and by (9.12) and (9.13)

$$F_{\text{left}} \geq c \sum_{\alpha \neq 0} \sigma^{|\alpha|} Q^{(\alpha)}(a^*) R_{\alpha} Q^{(\alpha)}(a), \quad (9.17a)$$

$$F_{\text{right}} \geq c \sum_{\alpha \neq 0} \sigma^{|\alpha|} Q^{(\alpha)}(a) R_{\alpha} Q^{(\alpha)}(a^*). \quad (9.17b)$$

Now for any term in F_{left} we decompose using the symmetry $P_{JK} = P_{KJ}$

$$\begin{aligned} & \partial_J Q(a^*) P_{JK} \partial_K Q(a) - [\partial_J Q(a^*), P_{JK}] \partial_K Q(a) + P_{JK} [\partial_K Q(a), \partial_J Q(a^*)] \\ &= \partial_K Q(a) P_{KJ} \partial_J Q(a^*) - [\partial_K Q(a), P_{JK}] \partial_J Q(a^*), \end{aligned}$$

and write this formula as

$$T_{m,J,K}^{\text{left}} = T_{m,J,K}^{\text{right}}.$$

It suffices to show that for all large σ and all small ϵ

$$\sum_{m,J,K} (m!)^{-1} \text{Re} (T_{m,J,K}^{\text{left}}) \leq C F_{\text{left}}, \quad (9.18a)$$

$$\sum_{m,J,K} (m!)^{-1} \text{Re} (T_{m,J,K}^{\text{right}}) \geq \frac{1}{2} F_{\text{right}}. \quad (9.18b)$$

The proof of (9.18a) and (9.18b) is given by using (9.17a) and (9.17b), respectively. Let us here derive (9.18a) only.

For the middle term we calculate using (9.4b)

$$-[\partial_J Q(a^*), P_{JK}] = \sum_{\alpha \neq 0} \frac{(-1)^{\alpha}}{\alpha!} \partial^{\alpha} \partial_J Q(a^*) \text{ad}_{a^*}^{\alpha} P_{JK}, \quad (9.19)$$

which gives

$$\begin{aligned} & - \sum_{m,J,K} (m!)^{-1} \text{Re} ([\partial_J Q(a^*), P_{JK}] \partial_K Q(a)) \\ & \leq C \sigma^{m+1/2} \sum_{m,J,K,\alpha \neq 0} \partial^{\alpha} \partial_J Q(a^*) r^{-(m+3|\alpha|/2)} \partial^{\alpha} \partial_J Q(a) \\ & \quad + C \sigma^{m-1/2} \sum_{m,J,K,\alpha \neq 0} \partial_K Q(a^*) r^{-(m+|\alpha|/2)} \partial_K Q(a) \\ & \leq \frac{1}{4} F_{\text{left}} + \frac{1}{4} F_{\text{left}}. \end{aligned} \quad (9.20)$$

In the last step we used (9.17a) and needed large σ large and ϵ small. It remains to consider the last term. Using (9.3) we have

$$\begin{aligned} & \sum_{m,J,K} (m!)^{-1} \text{Re} (P_{JK} [\partial_J Q(a^*), \partial_K Q(a)]) \\ &= \sum_{m,J,K} (m!)^{-1} \sum_{l \geq 1, J'_l, K'_l} (l!)^{-1} \text{Re} (P_{JK} \partial_{J'_l} \partial_J Q(a^*) P_{J'_l, K'_l} \partial_{J'_l} \partial_J Q(a)) + E', \end{aligned}$$

where E' comes from E in (9.3). Once P_{JK} is commuted past $\partial_{J'_l} \partial_J Q(a^*)$ we get for the fixed m and l portion of the summation in the first term on the right side

$$C_{m,l} \sum_{J,K,J'_l,K'_l} \partial_{J'_l} \partial_J Q(a^*) P_{J,K} P_{J'_l,K'_l} \partial_{J'_l} \partial_J Q(a) = C_{m,l} \sum_{L,M} \partial_L Q(a^*) P_{L,M} \partial_M Q(a),$$

where $L = (j_1, \dots, j_{l+m})$ and $M = (k_1, \dots, k_{l+m})$ and the j'_i 's and k'_i 's are summed over. The contribution from the resulting expression can be estimated by a multiple of F_{left} . The contribution from the commutator and the term E' are handled as in (9.20). Thus combining with (9.20) we obtain (9.18a).

9.4. **Proof of Theorem 1.5.** Let $f_m = r^{-(1+\epsilon)m/2}$. We first note that using the same ideas (commutation and the Cauchy-Schwarz inequality) as in the last two subsections we can equivalently write (for large σ , small enough ϵ , and some $C > 0$)

$$C[Q(a), Q(a^*)] \geq S; \quad (9.21)$$

$$S = \sum_{m=1} \sigma^m \sum_{l_1, \dots, l_m \leq d} \left(|(\partial_{l_1} \cdots \partial_{l_m} Q(a^*)) f_m(r)|^2 + |(\partial_{l_1} \cdots \partial_{l_m} Q(a)) f_m(r)|^2 \right).$$

We need a more efficient extraction of positivity from (9.21) than is immediately evident from this lower bound. We will also need a formula for $[Q(a), V_1]$ different from (9.15) which was used in the proof of Theorem 1.4.

Thus for $Q(\xi) = \xi^2$, we have $\partial_j Q(\xi) = 2\xi_j$ so that

$$\begin{aligned} S &= \Sigma_j 4\sigma f_1(a_j^* a_j + a_j a_j^*) f_1 + 8d\sigma^2 f_2^2 \\ &= 8\sigma f_1(p^2 + \sigma^2 \omega^2) f_1 + 8d\sigma^2 f_2^2. \end{aligned}$$

Thus for large σ and some $C > 0$

$$CS \geq \sigma^2 f_1^2. \quad (9.22)$$

Moving on to the commutator of $Q(a)$ with V_1 we have

$$\operatorname{Re} [Q(a), V_1] = \operatorname{Re} \Sigma_j [a_j [a_j, V_1] + [a_j, V_1] a_j] = -2\sigma \omega \cdot \nabla V_1. \quad (9.23)$$

Again applying (9.14), the result for $Q(\xi) = \xi^2$ follows from (9.22) and (9.23).

We now consider $Q(\xi) = (\xi^2)^2$. Note that $\partial_j Q(\xi) = 4\xi^2 \xi_j$ and $\partial_j^2 Q(\xi) = 8(\xi_j^2 + \xi^2/2)$. Whence for any operator $P \geq 0$

$$64^{-1} \Sigma_j (\partial_j^2 Q(a) P \partial_j^2 Q(a^*) + \partial_j^2 Q(a^*) P \partial_j^2 Q(a)) \geq \Sigma_j (a_j^2 P (a_j^*)^2 + (a_j^*)^2 P a_j^2).$$

We will also use the following identity for an operator b

$$\begin{aligned} &b^2 (b^*)^2 + (b^*)^2 b^2 \\ &= \left(b (b b^* + b^* b) b^* + b^* (b b^* + b^* b) b + \operatorname{ad}_b^2 (b^*) b^* + \operatorname{ad}_{b^*}^2 (b) b + [b, b^*]^2 \right) / 2. \end{aligned}$$

Applied to $P = I$ and $b = a_j$ it follows that

$$\begin{aligned} &64^{-1} \Sigma_j (\partial_j^2 Q(a) \partial_j^2 Q(a^*) + \partial_j^2 Q(a^*) \partial_j^2 Q(a)) \\ &\geq \Sigma_j (a_j (p_j^2 + \sigma^2 \omega_j^2) a_j^* + a_j^* (p_j^2 + \sigma^2 \omega_j^2) a_j + i\sigma \partial_j^2 \omega_j (a_j - a_j^*) + 2\sigma^2 (\partial_j \omega_j)^2) \\ &\geq 2\Sigma_j (\sigma^4 \omega_j^4 + \sigma^2 \partial_j (\omega_j \partial_j \omega_j)). \end{aligned}$$

If we add a suitable multiple of the $m = 4$ term of (9.21) we obtain

$$CS \geq \sigma^4 f_2^2. \quad (9.24)$$

We now go on to compute $[Q(a), V_1]$. We have

$$\begin{aligned} [(a^2)^2, V_1] &= 2\Sigma_j ([a_j, V_1] a_j a^2 + a^2 a_j [a_j, V_1]) + \Sigma_{i,j} ((\operatorname{ad}_{a_j}^2 V_1) a_i^2 - a_i^2 (\operatorname{ad}_{a_j}^2 V_1)) \\ &= -\frac{i}{2} \Sigma_j (\partial_j V_1 \partial_j Q(a) + \partial_j Q(a) \partial_j V_1) + \Sigma_i (a_i^2 (\Delta V_1) - (\Delta V_1) a_i^2). \end{aligned}$$

We bound

$$\begin{aligned} &-\operatorname{Im} \Sigma_j (\partial_j V_1 \partial_j Q(a) + \partial_j Q(a) \partial_j V_1) \\ &\leq \Sigma_j (\partial_j Q(a^*) f_1^2 \partial_j Q(a) + \partial_j Q(a) f_1^2 \partial_j Q(a^*) + (f_1^{-1} \partial_j V_1)^2) \\ &\leq C\sigma^{-1} S, \end{aligned}$$

where we have taken ϵ small, σ large and used (9.24). Similarly

$$\begin{aligned} & -2\operatorname{Re} \Sigma_i(a_i^2(\Delta V_1) + (\Delta V_1)a_i^2) \\ & \leq \Sigma_i((a_i^*)^2 f_2^2 a_i^2 + a_i^2 f_2^2 (a_i^*)^2) + 2d(f_2^{-1} \Delta V_1)^2 \\ & \leq 64^{-1} \Sigma_i(\partial_i^2 Q(a^*) f_2^2 \partial_i^2 Q(a) + \partial_i^2 Q(a) f_2^2 \partial_i^2 Q(a^*)) + 2d(f_2^{-1} \Delta V_1)^2 \\ & \leq C\sigma^{-2}S. \end{aligned}$$

Putting these estimates together gives Theorem 1.5 for $Q(\xi) = (\xi^2)^2$.

9.4.1. *Limits of the method, examples.* We continue the discussion of the examples treated above. Introduce $\langle \xi \rangle_\sigma = (\xi^2 + \sigma^2 \omega^2)^{1/2}$ and $\langle p \rangle_\sigma = (p^2 + \sigma^2 \omega^2)^{1/2}$. For $Q(\xi) = \xi^2$ we found the lower bound

$$CS \geq \sigma f_1 \langle p \rangle_\sigma^2 f_1 + \sigma^2 f_2^2. \quad (9.25)$$

For $Q(\xi) = (\xi^2)^2$ we have the lower bound

$$CS \geq \sigma^2 f_2 \langle p \rangle_\sigma^4 f_2 + \sigma^4 f_4^2, \quad (9.26a)$$

which is an extension of (9.24) and follows from its proof.

Letting

$$g = r^{-2} dx^2 + (\xi^2 + \sigma^2)^{-1} d\xi^2; \quad \sigma > 1,$$

the symbol of S for $Q(\xi) = \xi^2$ is in the (uniform parameter-dependent) class

$$S(\sigma r^{-1}(\xi^2 + \sigma^2), g),$$

and for $Q(\xi) = (\xi^2)^2$ in

$$S(\sigma r^{-1}(\xi^2 + \sigma^2)^3, g).$$

Whence in both cases the corresponding bounds are uniform in the parameter $\sigma > 1$. Comparing with (9.25) and (9.26a) we see that essentially we got an *elliptic* estimate in the case of $Q(\xi) = \xi^2$ (there is a loss of the small power r^ϵ and a slight modification at the critical point $x = 0$), while we only got a *subelliptic* estimate in the case of $Q(\xi) = (\xi^2)^2$. In the latter case possibly ‘‘ellipticity’’ would be the stronger bound

$$CS \geq \sigma f_1 \langle p \rangle_\sigma^6 f_1 + \sigma^4 f_4^2. \quad (9.26b)$$

Somehow we lost a factor of $r^{1+\epsilon} \sigma^{-1} \langle p \rangle_\sigma^2 \approx r \sigma^{-1} \langle p \rangle_\sigma^2$, and it is natural to ask if (9.26a) can be improved perhaps up to the optimal type bound (9.26b)? We will show this is not possible, in particular we will show that our bound (9.26a) can be considered ‘‘optimal’’. Note that the bound (9.26b) would lead to

$$CS \geq \sigma^7 |\omega|^6 r^{-1-\epsilon}, \quad (9.26c)$$

while (9.26a) implies

$$CS \geq \sigma^6 |\omega|^4 r^{-2-2\epsilon}. \quad (9.26d)$$

Lemma 9.1. *Consider $Q(\xi) = (\xi^2)^2$. Both of the following assertions are false.*

For some $s \in \mathbb{R}$ and $t \geq 0$ there exists $\epsilon_0 \in (0, 1)$ such that for all $\epsilon \in (0, \epsilon_0]$ there are constants $C_\epsilon, \sigma_\epsilon > 1$:

$$C_\epsilon [Q(a), Q(a^*)] \geq \sigma^{1+s} |\omega|^t r^{-2+\epsilon} \text{ for all } \sigma \geq \sigma_\epsilon. \quad (9.27a)$$

For some $s > 5$ and $t \geq 0$ there exists $\epsilon_0 \in (0, 1)$ such that for all $\epsilon \in (0, \epsilon_0]$ there are constants $C_\epsilon, \sigma_\epsilon > 1$:

$$C_\epsilon[Q(a), Q(a^*)] \geq \sigma^{1+s} |\omega|^t r^{-2} \text{ for all } \sigma \geq \sigma_\epsilon. \quad (9.27b)$$

Proof. We introduce a state of the form

$$\psi_\sigma(x) = k^{-(d-1)/2} Y_l(\hat{x}) \phi((|x| - k)/m),$$

where Y_l is a spherical harmonic and the indices $k, l, m > 0$ are large. More precisely we take $k = \sigma^{(5+\epsilon+|s|)/\epsilon}$, $m = \sqrt{k}/\sigma$ and l to be the integer part of \tilde{l} which is the unique positive solution to the equation

$$\frac{\tilde{l}(\tilde{l}+d-2)}{k^2} = \sigma^2 \omega(ke)^2,$$

where e is an arbitrary unit vector in \mathbb{R}^d . Fix $\phi \in C_c^\infty(\mathbb{R}_+)$ normalized, $\|\phi\|_{L^2} = 1$. Note that ψ_σ defined this way is approximately normalized.

Corresponding to (9.27a) and (9.27b)

$$\langle \sigma^{1+s} |\omega|^t r^{-2+\epsilon} \rangle_{\psi_\sigma} \approx \sigma^{1+s} k^{-2+\epsilon}, \quad (9.28a)$$

$$\langle \sigma^{1+s} |\omega|^t r^{-2} \rangle_{\psi_\sigma} \approx \sigma^{1+s} k^{-2}. \quad (9.28b)$$

To calculate the expectation of the left hand side of (9.27a) (or (9.27b)) we use (9.3). The leading term of the commutator is

$$32\sigma(a^*)^2 \Sigma_{i,j} a_i^* (\partial_i \omega_j) a_j a^2,$$

which using the notation $p_\omega = 1/2(\omega \cdot p + p \cdot \omega)$ and the familiar formulas

$$\begin{aligned} p^2(f(|x|) \otimes Y_l(\hat{x})) &= \left(-f''(|x|) - \frac{d-1}{|x|} f'(|x|) + \frac{l(l+d-2)}{|x|^2} f(|x|) \right) \otimes Y_l(\hat{x}), \\ i[p^2, p_\omega] &= 2\Sigma_{i,j} p_i (\partial_i \omega_j) p_j - \frac{1}{2}(\Delta^2 r), \end{aligned}$$

leads to the upper bound

$$\begin{aligned} &\langle [Q(a), Q(a^*)] \rangle_{\psi_\sigma} \\ &\leq C\sigma (\| \langle p \rangle_\sigma r^{-1/2} (p^2 - \sigma^2 \omega^2) \psi_\sigma \|^2 + \sigma^2 \| \langle p \rangle_\sigma r^{-1/2} p_\omega \psi_\sigma \|^2) + C \| \sigma r^{-1} \langle p \rangle_\sigma^2 \psi_\sigma \|^2 \\ &\leq C\sigma^3 k^{-1} (\| (\frac{l(l+d-2)}{|x|^2} - \sigma^2 \omega^2) \psi_\sigma \|^2 + \sigma^2 m^{-2}) + C\sigma^6 k^{-2} \\ &\leq C\sigma^3 k^{-1} (\sigma^4 m^2 / k^2 + \sigma^2 m^{-2} + \sigma^3 k^{-1}). \end{aligned}$$

In combination with (9.27a)–(9.28b) we thus obtain the impossible bounds

$$3C\sigma^6 k^{-2} = C\sigma^3 k^{-1} (\sigma^4 m^2 / k^2 + \sigma^2 m^{-2} + \sigma^3 k^{-1}) \geq \begin{cases} \sigma^{1+s} k^{-2+\epsilon}, \\ \sigma^{1+s} k^{-2}. \end{cases}$$

□

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