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# DECAY OF EIGENFUNCTIONS OF ELLIPTIC PDE'S

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# DECAY OF EIGENFUNCTIONS OF ELLIPTIC PDE'S

I. HERBST AND E. SKIBSTED

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

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## 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  $V$  bounded and measurable and with  $\lim_{|x| \rightarrow \infty} V(x) = 0$ .

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.

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

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

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is by definition regular if  $\lambda$  is not a critical value of  $Q$ , that is if

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

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 decay rate for eigenfunctions, cf. previous works for the Laplacian [CT, FHH2O1, FHH2O2, FHH2O3] corresponding to the case  $Q(\xi) = \xi^2$ . In particular we give necessary (phase-space) conditions for a positive number  $\sigma$  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 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

$$Q(\xi + i\sigma\omega) = \lambda, \quad (1.2a)$$

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

Another major subject of this paper is absence of super-exponentially decaying eigenfunctions (corresponding to the case  $\sigma_c = \infty$ ), cf. [FHH2O1, 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  $\sigma_c$ . Let  $\text{Ran}Q = \{Q(\xi) \mid \xi \in \mathbb{R}^d\}$ . 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  $V(x) = o(1)$ .
- 2)  $\lambda \in \text{Ran}Q$  but  $\lambda$  is not a critical value of  $Q$  and in addition

$$\forall \alpha : \partial^\alpha V_1(x) = o(|x|^{-|\alpha|}),$$

$$V_2(x) = o(|x|^{-1}).$$

**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*

$$Q(\xi + i\sigma_c\omega) = \lambda. \quad (1.3)$$

*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  $\xi^2$ .

In a generic sense (see the remark following the theorem), the next result gives a more precise estimate on the decay of  $\phi$  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*

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

*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 8.4. 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 8.1 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  $\lambda$  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 [FHH2O2, FHH2O3].

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  $\xi^2$  and  $(\xi^2)^2$ . This follows readily by a little refinement of the improved bounds, so-called subelliptic estimates, see (8.25) and (8.26a).

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  $(x, \xi)$  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  $\tau$ . 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. Example,  $Q(\xi) - \lambda = G(\xi^2)$ .** The main object of this section is to gain some understanding of the consequences of (1.2a) and (1.2b) for  $\sigma > 0$ . For general  $Q$  these two equations are actually  $2 + 2(d - 1) = 2d$  real scalar equations for the  $2d$

variables  $\xi, \omega$ , and  $\sigma$ . We take  $\omega \in S^{d-1}$ . In the case at hand there is an overall rotational symmetry which implies that if  $(\xi, \omega, \sigma)$  is a solution then for any real orthogonal matrix  $R$ ,  $(R\xi, R\omega, \sigma)$  is also a solution. Let  $z = (\xi + i\sigma\omega)^2$ . We have two equations:

$$G(z) = 0, \quad (1.6)$$

$$P_{\perp}(\omega)\nabla_{\xi}Q(\xi + i\sigma\omega) = 2G'(z)P_{\perp}(\omega)\xi = 0. \quad (1.7)$$

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  $\leq \frac{q-2}{2}$  values of  $\lambda$ . If  $\lambda$  is not one of these at most  $\frac{q-2}{2}$  possible real numbers there are  $\leq q/2$  exceptional numbers. In the case of  $G(z) = z^2 - \lambda$ , involving the bilaplacian, if  $\lambda \neq 0$  there is exactly one solution with positive  $\sigma$ . 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  $Q(p) + V(x)$  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  $\phi$  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  $\phi$  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  $\xi^2$ , except for at most  $(q - 2)/2$  real  $\lambda$ 's,  $\sigma \in \Sigma_{\text{exc}}(\lambda)$  is sufficient for  $\sigma$  to be the critical decay rate of an eigenfunction with eigenvalue  $\lambda$  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. Notation and 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). Recalling  $q = \text{degree}(Q)$  obviously  $Q \in S(\langle \xi \rangle^q, g)$ .

Recall the  $L^2$ -boundedness result, here amounting to

$$a \in S(1, g) \Rightarrow \|\text{Op}^w(a)\| \leq C, \quad (1.8a)$$

where  $C \geq 0$  can be chosen independently of  $a$  from any bounded family of symbols in  $S(1, g)$  (i.e. any family for which each semi-norm has a uniform bound). A family of such symbols is said to be uniformly in  $S(1, g)$ . We shall use similar terminology for symbols in  $S(m, g)$ .

By the Fefferman-Phong inequality

$$a \in S(\langle x \rangle^2 \langle \xi \rangle^2, g), a \geq 0 \Rightarrow \text{Op}^w(a) \geq -C, \quad (1.8b)$$

where  $C \geq 0$  can be chosen independently of  $a$  from any bounded family of such symbols.

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

$$\chi_-^2 + \chi_+^2 = 1. \quad (1.9)$$

For any  $\kappa > 0$  we define  $\chi_-(t \leq \kappa) = \chi_-(t/\kappa)$  and  $\chi_+(t \geq \kappa) = \chi_+(t/\kappa)$ .

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  $\langle \psi, A\psi \rangle = \langle A \rangle_\psi$ .

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

$$r(x) = r_1(x) = \langle x \rangle. \quad (1.10a)$$

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

$$r(x) = r_\epsilon(x) = \langle x \rangle - \langle x \rangle^{1-\epsilon} + 1. \quad (1.10b)$$

Note that these are positive smooth strictly convex functions that at infinity behave as  $|x|$ . However while  $r_1$  tends to be degenerately convex at infinity (just as  $|x|$ ), this deficiency appears somewhat cured for  $r_\epsilon$  (in particular in the regime where  $\epsilon$  is small). In both cases we shall use the notation  $\omega = \omega(x) = \text{grad } r$ . The functions  $r_\epsilon$  were used in [RT] in a different context. See also [IS1].

## 2. IDEAS OF PROOF OF THEOREMS 1.2 AND 1.3

Consider the function  $r$  given by either (1.10a) or (1.10b).

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  $\phi$  is an eigenfunction with eigenvalue  $\lambda$ , 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 7 under the assumptions of Theorem 1.1.) So we consider an eigenfunction  $\phi$  with  $\phi_{\sigma_0} \in L^2$  for some  $\sigma_0 > 0$  and want to derive a priori bounds of  $\phi_\sigma$  for  $\sigma < \sigma_c$ . See (2.7) for an example of such bound.

The result Theorem 1.2 i) can be interpreted as an energy estimate which 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*  $A$  with Weyl symbol

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

Consider

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

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

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 rest of our discussion in this section we only discuss the proof of Theorem 1.3.

Let us note that 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 and (1.8b) we show that (2.5) is preserved under quantization and, more precisely, we derive a bound like

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

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. Thus we have converted (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) we obtain Theorem 1.3.

### 3. ELABORATION ON ENERGY LOCALIZATION

This section contains various preliminary bounds valid for any eigenfunction  $\phi$ ,  $(H - \lambda)\phi = 0$ , with  $\sigma_c > 0$ . These are, more precisely, a priori bounds on  $\phi_\sigma = e^{\sigma r}\phi$  for  $\sigma \in [0, \sigma_c)$ . Here  $r$  is the function given by either (1.10a) or (1.10b). The bounds are uniform in  $\sigma$  varying in any bounded subset of  $[0, \sigma_c)$ . In the last subsection we establish some uniform bounds for certain non-convex parameter-dependent approximations. In this section we shall only need boundedness of  $V$  (i.e. decay assumptions will not be needed).

**3.1. Sobolev regularity.** Let us note that

$$\forall \sigma \in [0, \sigma_c), s \in \mathbb{R} : \phi_\sigma \in r^{-s}H^q, \quad (3.1)$$

where  $H^q$  is the standard Sobolev space of order  $q$ ,

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

In fact letting  $f(r) = \sigma r + s \ln r$  we can write

$$e^f Q(p) e^{-f} = \text{Op}^w(a),$$

where  $a$  is an elliptic symbol in  $S(\langle \xi \rangle^q, g)$ , cf. Appendix A. Then (3.1) follows from

$$\text{Op}^w(a) r^s \phi_\sigma = r^s e^{\sigma r} (\lambda - V) \phi \in L^2.$$

**3.2. Energy bounds.** For  $s \in \mathbb{R}$  we calculate on the one hand

$$\|r^s(\tilde{X} + i\tilde{Y})\phi_\sigma\|^2 = \|r^s\tilde{X}\phi_\sigma\|^2 + \|r^s\tilde{Y}\phi_\sigma\|^2 - 2\text{Im}\langle \tilde{X}r^{2s}\tilde{Y} \rangle_{\phi_\sigma}, \quad (3.2a)$$

while on the other hand

$$\|r^s(\tilde{X} + i\tilde{Y})\phi_\sigma\|^2 = \|r^s V \phi_\sigma\|^2. \quad (3.2b)$$

Whence to get a useful bound we need to examine the last term to the right in (3.2a):

$$\begin{aligned} & -2\text{Im}\langle \tilde{X}r^{2s}\tilde{Y} \rangle_{\phi_\sigma} \\ & \geq \langle i[\tilde{X}, \tilde{Y}] \rangle_{r^s\phi_\sigma} - \frac{1}{5}(\|r^s\tilde{Y}\phi_\sigma\|^2 + \|r^s\tilde{X}\phi_\sigma\|^2) - C_1\|r^{s-1}\phi_\sigma\|^2 - C_1\|r^{s-1}\tilde{X}\phi_\sigma\|^2 \\ & \geq \langle i[\tilde{X}, \tilde{Y}] \rangle_{r^s\phi_\sigma} - \frac{1}{4}(\|r^s\tilde{Y}\phi_\sigma\|^2 + \|r^s\tilde{X}\phi_\sigma\|^2) - C_2\|r^{s-1}\phi_\sigma\|^2 - C_2\|V\phi\|^2. \end{aligned}$$

Here we used the ellipticity of  $Q(p)$  and  $\tilde{X}$  estimating, cf. (1.8b), like

$$r^t \langle p \rangle^{2q} r^t \leq C_{1,t} \tilde{X} r^{2t} \tilde{X} + C_{2,t} r^{2t}. \quad (3.3)$$

Using (1.8b), (2.3) and (3.3) we obtain

$$\begin{aligned} \langle i[\tilde{X}, \tilde{Y}] \rangle_{r^s \phi_\sigma} & \\ & \geq -C_1(\|r^{s-1} \tilde{X} \phi_\sigma\|^2 + \|r^{s-1} \phi_\sigma\|^2) \\ & \geq -\frac{1}{4} \|r^s \tilde{X} \phi_\sigma\|^2 - C_2 \|r^{s-1} \phi_\sigma\|^2 - C_2 \|V \phi\|^2. \end{aligned}$$

In combination with (3.2a) these bounds yield

$$\|r^s(\tilde{X} + i\tilde{Y})\phi_\sigma\|^2 \geq \frac{1}{2}(\|r^s \tilde{Y} \phi_\sigma\|^2 + \|r^s \tilde{X} \phi_\sigma\|^2) - C \|r^{s-1} \phi_\sigma\|^2 - C \|V \phi\|^2,$$

and therefore by (3.2b) that

$$\|r^s \tilde{Y} \phi_\sigma\|^2 + \|r^s \tilde{X} \phi_\sigma\|^2 \leq 2 \|r^s V \phi_\sigma\|^2 + C \|r^{s-1} \phi_\sigma\|^2 + C \|V \phi\|^2. \quad (3.4)$$

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

$$f_m = f_m(r) = r(\sigma + \gamma/(1 + r/m)); m \in \mathbb{N}. \quad (3.5)$$

We have in mind to use this construction for  $\sigma \in [0, \sigma_c)$  and small  $\gamma > 0$ . 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. In fact we need to modify (2.3), for example as

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

Here  $X$  and  $Y$  are defined in terms of  $f_m$  (rather than in terms of the exponent  $\sigma r$  as before),  $\omega(x) = \text{grad } r$ , and  $C > 0$  is independent of  $m$  and  $\gamma$ .

Using this bound we obtain the following modifications of (3.4), using the (slightly inconsistent) notation  $\phi_m = e^{f_m} \phi$ :

$$\|r^s \tilde{Y} \phi_m\|^2 + \|r^s \tilde{X} \phi_m\|^2 \leq 2 \|r^s V \phi_m\|^2 + C \|r^{s-1/2} \phi_m\|^2 + C \|V \phi\|^2. \quad (3.6)$$

The constants can be chosen to be independent of  $m \in \mathbb{N}$  and  $\gamma \in (0, 1]$ . We also note that (3.6) 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 will be needed in Section 7). Somewhat refined  $\gamma$ -dependent constants can be given, however this will not be needed.

#### 4. PROOF OF THEOREM 1.2 i)

Suppose (1.3) does not have any solution, i.e.

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

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 3.3. We arrive at a contradiction by showing the uniform bound

$$\|\phi_m\|^2 \leq C \|\phi\|^2; \phi_m = e^{f_m} \phi. \quad (4.1)$$

Indeed with a proper adjustment of  $\sigma$  and  $\gamma$  we have  $X^2 + Y^2 \geq \kappa$  for  $|x|$  large (by a continuity argument). Then by using (1.8b), (3.3) and (3.6) with  $s = 0$  we

obtain

$$\begin{aligned}\|\phi_m\|^2 &\leq C_1(\|(\tilde{X}^2 + \tilde{Y}^2)^{1/2}\phi_m\|^2 + \|r^{-1}\phi_m\|^2) \\ &\leq C_2(\|V\phi_m\|^2 + \|r^{-1/2}\phi_m\|^2).\end{aligned}\tag{4.2}$$

Clearly (4.1) follows from (4.2).

## 5. PROOF OF THEOREM 1.3

Let  $r = r_\epsilon$ , and let  $\omega = \omega(x) = \text{grad } r$ . Using Section 3 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  $\phi_\sigma = e^{\sigma r}\phi$  for  $\sigma < \sigma_c$ , but close, and want to prove (2.7).

We introduce

$$\hat{S}_{\sigma,\lambda} = \{(x, \xi) \in (\mathbb{R}^d \setminus \{0\}) \times \mathbb{R}^d | Q(\xi + i\sigma\hat{x}) = \lambda\},\tag{5.1}$$

which at infinity is close to the set  $S_{\sigma,\lambda}$  of (2.1). We localize near  $\hat{S}_{\sigma,\lambda}$  introducing a quantization, say  $\tilde{\chi}_-$ , of the symbols  $\chi_- = \chi_-(X^2 + Y^2 \leq \kappa)$ ,  $\kappa > 0$  small, see Subsection 1.3. We have (slightly inconsistently) shortened the notation suppressing the dependence of  $\kappa$ . Note in particular that we are going to use the decomposition of unity (1.9) for the  $\kappa$ -dependent partition functions.

Now we estimate using (1.8b), (3.3) and (3.4)

$$\begin{aligned}\|\tilde{\chi}_+\phi_\sigma\|^2 &\leq C_1(\|(\tilde{X}^2 + \tilde{Y}^2)^{1/2}\phi_\sigma\|^2 + \|r^{-1}\phi_\sigma\|^2) \\ &\leq C_2(\|V\phi_\sigma\|^2 + \|r^{-1}\phi_\sigma\|^2).\end{aligned}\tag{5.2a}$$

Using (3.3), (3.4) and (5.2a) we obtain the improvement

$$\begin{aligned}\|\langle p \rangle^q \tilde{\chi}_+\phi_\sigma\|^2 &\leq C_1\|\tilde{X}\tilde{\chi}_+\phi_\sigma\|^2 + C_2\|\tilde{\chi}_+\phi_\sigma\|^2 \\ &\leq C'_1\|\tilde{X}\phi_\sigma\|^2 + C'_2\|r^{-1}\phi_\sigma\|^2 + C_3\|Vr^{-1}\phi_\sigma\|^2 \\ &\quad + C_2\|\tilde{\chi}_+\phi_\sigma\|^2 \\ &\leq C(\|V\phi_\sigma\|^2 + \|r^{-1}\phi_\sigma\|^2).\end{aligned}\tag{5.2b}$$

Redoing the considerations in Section 2 we see that (2.5) is modified as

$$\begin{aligned}r\{X, Y\} + 2rY^2 + \{X, r\}Y &\geq r\{X, Y\} + rY^2 - C_1r^{-1}\langle \xi \rangle^{2q} \\ &\geq 2cr^{-\epsilon} + rY^2 - C_2\langle \xi \rangle^{2q}\chi_+^2.\end{aligned}$$

for small enough  $\kappa$ . We quantize, combine with (5.2b) and conclude

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

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

$$c\|r^{-\epsilon/2}\phi_\sigma\|^2 \leq -\langle i[V, A] \rangle_{\phi_\sigma} - \|r^{1/2}\tilde{Y}\phi_\sigma\|^2 + C\|\phi\|^2.\tag{5.3}$$

Using the conditions on  $V_1$  and  $V_2$  and (5.3), assuming also  $\epsilon < \min(\delta_1, 2\delta_2)$ , and again (3.3) and (3.4) we can show (2.7) as follows: We estimate

$$\begin{aligned} -\langle i[V_1, A] \rangle_{\phi_\sigma} &\leq C_1 \|\langle p \rangle^q r^{-\delta_1/2} \phi_\sigma\|^2 \leq C_2 \|r^{-\delta_1/2} \phi_\sigma\|^2, \\ -\langle i[V_2, A] \rangle_{\phi_\sigma} &\leq C_1 \|r^{-\delta_2} \phi_\sigma\|^2 + \|r^{1/2} \tilde{Y} \phi_\sigma\|^2 + C_2 \|r^{-1/2} \phi_\sigma\|^2, \end{aligned}$$

and insert into (5.3) leading to the uniform bound

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

Now take  $\sigma \nearrow \sigma_c$ .

## 6. 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  $(\omega, \xi)$  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 toward the following analogue of (2.7) which we will show to be uniform in  $\sigma < \sigma_c$ :

$$\|\phi_\sigma\|^2 \leq C \|\phi\|^2. \quad (6.1)$$

Let  $\hat{S}_{\sigma, \lambda}$  be defined by (5.1). By continuity and compactness we have uniformly in  $\sigma$  close to  $\sigma_c$ ,

$$\begin{aligned} &\nabla_\xi X(\xi + i\sigma \hat{x}) P_\perp(\hat{x}) \nabla_\xi X(\xi + i\sigma \hat{x}) \\ &+ \nabla_\eta X(\xi + i\sigma \hat{x}) P_\perp(\hat{x}) \nabla_\eta X(\xi + i\sigma \hat{x}) \geq k > 0 \end{aligned} \quad (6.2)$$

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

In fact this is valid in a neighbourhood of  $\hat{S}_{\sigma_c, \lambda}$ , and we can also freely replace  $\hat{x}$  by  $\omega(x)$  in (6.2) (since only large  $|x|$  matters below). In particular we have the following version of (2.5) in a neighbourhood of  $S_{\sigma, \lambda} \cap \{r > R\}$  for  $R > 1$  sufficiently large:

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

Using (3.3), (3.4) and the procedure of Section 5 we obtain, cf. (5.2b),

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

We continue mimicking Section 5 and come to the following analogue of (5.3) (using now only that  $V = o(|x|^0)$ )

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

and from this indeed (6.1). Next we take  $\sigma \nearrow \sigma_c$ , and we conclude that  $e^{\sigma|x|} \phi \in L^2$  with  $\sigma = \sigma_c$ .

The next step is to use Subsection 3.3 to show that  $e^{\sigma|x|} \phi \in L^2$  with  $\sigma$  slightly bigger, which obviously is a contradiction. We mimic Section 4. 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 3.3 and consider the corresponding state  $\phi_m = e^{f_m} \phi$ . Using (3.3) and (3.6) with  $s = 0$  mimicking Section 5 we obtain the following version of (5.3)

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

Estimating the commutator as before we arrive at the estimate

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

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

## 7. 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  $\sigma_c > 0$ . We omit the details.

Otherwise take  $\sigma = 0$  and  $r = r_1$  in (3.5). Whence we consider  $f_m := \gamma r(1+r/m)^{-1}$ ,  $m \in \mathbb{N}$ . Let the number  $\gamma \in (0, 1]$  be taken small. Under the conditions 2) of Theorem 1.1 and abbreviating  $\phi_m = e^{f_m} \phi$  we shall prove the estimate

$$\|\phi_m\|^2 \leq C\|\phi\|^2, \quad (7.1)$$

for small enough  $\gamma$ . Taking  $m \rightarrow \infty$  completes the proof of Theorem 1.1.

Clearly

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

We consider the symbols  $X_m$  and  $Y_m$  given by conjugation by  $e^{f_m}$  (in agreement with the previous sections). 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: Letting

$$a_m(x, \xi) = (r/\gamma g_m(r)) Y_m(x, \xi)$$

we note that  $a_m \in S(r\langle \xi \rangle^q, g)$  uniformly in  $m$  (see Subsection 1.3 for terminology). Introduce partition functions  $\chi_{-,m} = \chi_-(X_m^2 + Y_m^2 \leq \kappa)$  and  $\chi_{+,m} = \chi_+(X_m^2 + Y_m^2 \geq \kappa)$  for (small)  $\kappa > 0$ . Indeed we can estimate for small  $\kappa, \gamma > 0$  using the assumptions

$$\{X_m, a_m\} + 2a_m Y_m \geq 2c - C\langle \xi \rangle^{2q} \chi_{+,m}^2$$

for constants  $c, C > 0$  being independent of  $m$ . Here we use that

$$\{X_m, a_m\} = |\nabla Q(\xi)|^2 + \gamma a_{0,\gamma,m} + a_{-1,\gamma,m},$$

where  $a_{0,\gamma,m} \in S(\langle \xi \rangle^q, g)$  and  $a_{-1,\gamma,m} \in S(r^{-1}\langle \xi \rangle^q, g)$ , both uniformly in  $\gamma$  and  $m$ , and we use that  $2a_m Y_m \geq 0$ . We quantize yielding the bound (dropping indices)

$$\text{Im}(A(\tilde{X} + i\tilde{Y})) \geq c - \text{Re}(B(\tilde{X} + i\tilde{Y})) - Cr^{-1/2} \langle p \rangle^{2q} r^{-1/2}, \quad (7.2)$$

where the symbol of  $B$  is in  $S(\langle \xi \rangle^q, g)$  uniformly in  $m$ , and the constants  $c, C > 0$  are independent of  $m$ , cf. Appendix A.

Now we apply (7.2) to the state  $\phi_{m,n} := \chi_-(r \leq n) \phi_m$ . Taking  $n \rightarrow \infty$  by using Lebesgue's dominated convergence theorem leaves us with

$$\langle \frac{i}{2}[A, V_1] \rangle_{\phi_m} - \text{Im} \langle r^{-1} A \phi_m, r V_2 \phi_m \rangle - \text{Re} \langle B^* \phi_m, V \phi_m \rangle \geq \langle c - Cr^{-1/2} \langle p \rangle^{2q} r^{-1/2} \rangle_{\phi_m}.$$

Next we use the Cauchy-Schwarz inequality yielding the following bound for any (small)  $\varepsilon > 0$

$$C_\varepsilon \|\langle p \rangle^q \phi\|^2 \geq \frac{1}{2} c \|\phi_m\|^2 - \varepsilon \|\langle p \rangle^q \phi_m\|^2.$$

Finally we invoke (3.3) and (3.6) with  $t = s = 0$  yielding (7.1).

## 8. PROOF OF THEOREMS 1.4 AND 1.5

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

$$a = (a_1, \dots, a_d) = e^{-\sigma r} p e^{\sigma r} = p - i\sigma\omega, \quad (8.1)$$

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”

$$[Q(a), Q(a^*)] \approx 2\sigma Q'(a)\omega'Q'(a^*)^T \geq 0. \quad (8.2)$$

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 8.4.1 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 (8.2) 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.

**8.1. 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:

$$[Q(a), Q(a^*)] = F + E; \quad (8.3)$$

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

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

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  $\sigma$  large, the term  $E$  will be seen to be negligible.

To prove (8.3) 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  $\text{ad}_{b_1}$ ,  $\text{ad}_{b_2}$ ,  $r_{b_1}$ ,  $r_{b_2}$ ,  $l_{b_1}$ ,  $l_{b_2}$  commute. For  $f$  a polynomial in  $d$  variables and  $b_1, b_2, \dots, b_d$  commuting operators, we note the Taylor type formulas

$$\begin{aligned} [f(b), c] &= (f(\text{ad}_b + r_b) - f(r_b))c \\ &= \sum_{\alpha \neq 0} (\alpha!)^{-1} \text{ad}_b^\alpha(c) \partial^\alpha f(b), \end{aligned} \quad (8.4a)$$

$$\begin{aligned} [f(b), c] &= (f(l_b) - f(-\text{ad}_b + l_b))c \\ &= \sum_{\alpha \neq 0} \frac{(-1)^{|\alpha|+1}}{\alpha!} \partial^\alpha f(b) \text{ad}_b^\alpha(c). \end{aligned} \quad (8.4b)$$

We will also need the Leibniz type formula

$$\text{ad}_b^\alpha(cd) = \sum_{\gamma} \binom{\alpha}{\gamma} \text{ad}_b^{\alpha-\gamma}(c) \text{ad}_b^\gamma(d). \quad (8.5)$$

By (8.4a) and (8.4b)

$$[Q(a), Q(a^*)] = \sum_{\alpha \neq 0} (\alpha!)^{-1} (\text{ad}_a^\alpha Q(a^*)) Q^{(\alpha)}(a), \quad (8.6)$$

$$[a_j, Q(a^*)] = \sum_{\alpha \neq 0} \frac{(-1)^\alpha}{\alpha!} Q^{(\alpha)}(a^*) \text{ad}_{a^*}^\alpha a_j. \quad (8.7)$$

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

$$\sum_{\alpha \neq 0} f(\alpha) = \sum_{\beta, k} \zeta(\beta + e_k) f(\beta + e_k), \quad (8.8)$$

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  $(\beta, k)$  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

$$\text{ad}_a^{\alpha+e_j} Q(a^*) = \sum_{\beta, \gamma, \mu, k, \gamma+\mu=\alpha} \frac{\text{ad}_a^\mu Q^{(\beta+e_k)}(a^*)}{\mu!} \left\{ (-1)^\beta d(\beta + e_k) \frac{\alpha!}{\gamma!} \text{ad}_a^{\beta+\gamma} p_{jk} \right\}. \quad (8.9)$$

Here we used (8.5), (8.7), (8.8), 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

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

$$\begin{aligned} & \sum_{\mu \neq 0} \frac{\text{ad}_a^\mu Q(a^*)}{\mu!} f(\mu) \\ &= \sum_{\beta, \gamma, j, k, \mu} \frac{\text{ad}_a^\mu Q^{(\beta+e_k)}(a^*)}{\mu!} \left\{ (-1)^\beta \lambda(\beta, \gamma, \mu, j, k) \text{ad}_a^{\beta+\gamma} (p_{jk}) f(\gamma + \mu + e_j) \right\} \\ &= \sum_{\beta, \gamma, j, k} Q^{(\beta+e_k)}(a^*) \left\{ (-1)^\beta d(\beta + e_k) d(\gamma + e_j) \text{ad}_a^{\beta+\gamma} (p_{jk}) f(\gamma + e_j) \right\} \\ & \quad + \sum_{\beta, \gamma, j, k} \sum_{\mu \neq 0} \frac{\text{ad}_a^\mu Q^{(\beta+e_k)}(a^*)}{\mu!} \left\{ (-1)^\beta \lambda(\beta, \gamma, \mu, j, k) \text{ad}_a^{\beta+\gamma} (p_{jk}) f(\gamma + e_j + \mu) \right\}. \end{aligned} \quad (8.10)$$

Here we have used (8.8) and (8.9).



From (8.10) 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  $\Gamma_l$  are multi-indices, while the components of  $J_l$  and  $K_l$  are numbers in  $\{1, \dots, d\}$ .

Repeatedly using (8.10) we obtain

$$\begin{aligned} [Q(a), Q(a^*)] &= \sum_{\beta, \gamma, j, k} d(\beta + e_k) d(\gamma + e_j) (D^{(\beta+e_k)} Q)(a)^* p_{jk\beta\gamma} (D^{(\gamma+e_j)} Q)(a) \quad (8.11) \\ &+ \sum_{m \geq 2, B_m, \Gamma_m, J_m, K_m} C_{J_m, K_m}^{B_m, \Gamma_m} (D^{\sum_{l=1}^m (\beta_l + e_{k_l})} Q)(a)^* \left( \prod_{l=1}^m p_{j_l k_l \beta_l \gamma_l} \right) (D^{\sum_{l=1}^m (\gamma_l + e_{j_l})} Q)(a). \end{aligned}$$

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 (8.3) note that in (8.11) we can replace  $C_{J_m}$  by its average over permutations. To compute this we use (8.8) 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 (8.3) with  $E$  given with reference to (8.11).

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

$$P \otimes \cdots \otimes P \geq c\sigma^m r^{-(1+\epsilon)m} I \quad (8.12)$$

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

$$CF \geq \sum_{\alpha \neq 0} \sigma^{|\alpha|} \partial^\alpha Q(a^*) r^{-(1+\epsilon)|\alpha|} \partial^\alpha Q(a). \quad (8.13)$$

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  $\mu$  or  $\nu$  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  $\sigma$ . It follows that  $E$  is negligible compared to  $F$  for large  $\sigma$ .

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

$$\begin{aligned} (\phi_\sigma, [Q(a), Q(a^*)]\phi_\sigma) + 2\operatorname{Re}(\phi_\sigma, [Q(a), V_1]\phi_\sigma) + \|(Q(a) + V_1 - \lambda)\phi_\sigma\|^2 \\ = \|V_2\phi_\sigma\|^2. \end{aligned} \quad (8.14)$$

We use (8.4a) to compute  $[Q(a), V_1]$ :

$$\begin{aligned} [Q(a), V_1] &= \sum_{\alpha \neq 0} (\alpha!)^{-1} (\operatorname{ad}_a^\alpha V_1) \partial^\alpha Q(a) \\ &= \sum_{\alpha \neq 0} (\alpha!)^{-1} ((-i\partial)^\alpha V_1) \partial^\alpha Q(a). \end{aligned} \quad (8.15)$$

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  $\epsilon$  small and then using the formula (8.13). In addition the terms with  $m = q$  in (8.13) 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.

8.3. **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  $\sigma$

$$C[Q(a), Q(a^*)] \geq \sum_{\alpha \neq 0} \sigma^{|\alpha|} (Q^{(\alpha)}(a^*) R_\alpha Q^{(\alpha)}(a) + Q^{(\alpha)}(a) R_\alpha Q^{(\alpha)}(a^*)). \quad (8.16)$$

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 (8.12) and (8.13)

$$F_{\text{left}} \geq c \sum_{\alpha \neq 0} \sigma^{|\alpha|} Q^{(\alpha)}(a^*) R_{\alpha} Q^{(\alpha)}(a), \quad (8.17a)$$

$$F_{\text{right}} \geq c \sum_{\alpha \neq 0} \sigma^{|\alpha|} Q^{(\alpha)}(a) R_{\alpha} Q^{(\alpha)}(a^*). \quad (8.17b)$$

Now for any term in  $F_{\text{left}}$  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  $\sigma$  and all small  $\epsilon$

$$\sum_{m,J,K} (m!)^{-1} \text{Re} (T_{m,J,K}^{\text{left}}) \leq C F_{\text{left}}, \quad (8.18a)$$

$$\sum_{m,J,K} (m!)^{-1} \text{Re} (T_{m,J,K}^{\text{right}}) \geq \frac{1}{2} F_{\text{right}}. \quad (8.18b)$$

The proof of (8.18a) and (8.18b) is given by using (8.17a) and (8.17b), respectively. Let us here derive (8.18a) only.

For the middle term we calculate using (8.4b)

$$-[\partial_J Q(a^*), P_{JK}] = \sum_{\alpha \neq 0} \frac{(-1)^{\alpha}}{\alpha!} \partial^{\alpha} \partial_J Q(a^*) \text{ad}_{a^*}^{\alpha} P_{JK}, \quad (8.19)$$

which gives

$$\begin{aligned} & - \sum_{m,J,K} (m!)^{-1} \text{Re} ([\partial_J Q(a^*), P_{JK}] \partial_K Q(a)) \\ & \leq C \sigma^{m+1/2} \sum_{m,J,K,\alpha \neq 0} \partial^{\alpha} \partial_J Q(a^*) r^{-(m+3|\alpha|/2)} \partial^{\alpha} \partial_J Q(a) \\ & \quad + C \sigma^{m-1/2} \sum_{m,J,K,\alpha \neq 0} \partial_K Q(a^*) r^{-(m+|\alpha|/2)} \partial_K Q(a) \\ & \leq \frac{1}{4} F_{\text{left}} + \frac{1}{4} F_{\text{left}}. \end{aligned} \quad (8.20)$$

In the last step we used (8.17a) and needed large  $\sigma$  large and  $\epsilon$  small. It remains to consider the last term. Using (8.3) 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 (8.3). 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  $F_{\text{left}}$ . The contribution from the commutator and the term  $E'$  are handled as in (8.20). Thus combining with (8.20) we obtain (8.18a).

8.4. **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  $\sigma$ , small enough  $\epsilon$ , and some  $C > 0$ )

$$C[Q(a), Q(a^*)] \geq S; \quad (8.21)$$

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

We need a more efficient extraction of positivity from (8.21) than is immediately evident from this lower bound. We will also need a formula for  $[Q(a), V_1]$  different from (8.15) 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  $\sigma$  and some  $C > 0$

$$CS \geq \sigma^2 f_1^2. \quad (8.22)$$

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

$$\operatorname{Re} [Q(a), V_1] = \operatorname{Re} \Sigma_j [a_j [a_j, V_1] + [a_j, V_1] a_j] = -2\sigma \omega \cdot \nabla V_1. \quad (8.23)$$

Again applying (8.14), the result for  $Q(\xi) = \xi^2$  follows from (8.22) and (8.23).

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 (8.21) we obtain

$$CS \geq \sigma^4 f_2^2. \quad (8.24)$$

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  $\epsilon$  small,  $\sigma$  large and used (8.24). 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  $Q(\xi) = (\xi^2)^2$ .

8.4.1. *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

$$CS \geq \sigma f_1 \langle p \rangle_\sigma^2 f_1 + \sigma^2 f_2^2. \quad (8.25)$$

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

$$CS \geq \sigma^2 f_2 \langle p \rangle_\sigma^4 f_2 + \sigma^4 f_4^2, \quad (8.26a)$$

which is an extension of (8.24) 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 (cf. [Hö, Chapt. XVIII])

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

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

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

Comparing with (8.25) and (8.26a) 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  $r^\epsilon$  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

$$CS \geq \sigma f_1 \langle p \rangle_\sigma^6 f_1 + \sigma^4 f_4^2. \quad (8.26b)$$

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 (8.26a) can be improved perhaps up to the optimal type bound (8.26b)? We will show this is not possible, in particular we will show that our bound (8.26a) can be considered “optimal”. Note that the bound (8.26b) would lead to

$$CS \geq \sigma^7 |\omega|^6 r^{-1-\epsilon}, \quad (8.26c)$$

while (8.26a) implies

$$CS \geq \sigma^6 |\omega|^4 r^{-2-2\epsilon}. \quad (8.26d)$$

**Lemma 8.1.** *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  $C_\epsilon, \sigma_\epsilon > 1$ :*

$$C_\epsilon [Q(a), Q(a^*)] \geq \sigma^{1+s} |\omega|^t r^{-2+\epsilon} \text{ for all } \sigma \geq \sigma_\epsilon. \quad (8.27a)$$

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  $C_\epsilon, \sigma_\epsilon > 1$ :

$$C_\epsilon [Q(a), Q(a^*)] \geq \sigma^{1+s} |\omega|^t r^{-2} \text{ for all } \sigma \geq \sigma_\epsilon. \quad (8.27b)$$

*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

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

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  $\psi_\sigma$  defined this way is approximately normalized.

Corresponding to (8.27a) and (8.27b)

$$\langle \sigma^{1+s} |\omega|^t r^{-2+\epsilon} \rangle_{\psi_\sigma} \approx \sigma^{1+s} k^{-2+\epsilon}, \quad (8.28a)$$

$$\langle \sigma^{1+s} |\omega|^t r^{-2} \rangle_{\psi_\sigma} \approx \sigma^{1+s} k^{-2}. \quad (8.28b)$$

To calculate the expectation of the left hand side of (8.27a) (or (8.27b)) we use (8.3). The leading term of the commutator is

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

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

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

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 (8.27a)–(8.28b) we thus obtain the impossible bounds

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

□

## APPENDIX A. THE WEYL SYMBOL OF $Q(p + i\nabla f(x))$

We give a combinatorial formula for the Weyl symbol of

$$\text{Op}^w(b) := e^{f(x)} \text{Op}^w(a) e^{-f(x)},$$

namely formally

$$b(x, \xi) = a(x, \xi - i\nabla_y) \exp(f(x - y/2) - f(x + y/2))|_{y=0}. \quad (A.1)$$

In the special case that  $a(x, \xi)$  is a polynomial,  $Q(\xi)$ , and  $f \in C^\infty(\mathbb{R}^n)$  we have

$$\begin{aligned}
b(x, \xi) &= e^{-i\nabla_\xi \cdot \nabla_y} e^{f(x-y/2) - f(x+y/2)} \Big|_{y=0} Q(\xi) \\
&= e^{f(x+i\nabla_\xi/2) - f(x-i\nabla_\xi/2)} Q(\xi) \\
&= Q(\xi) + \sum_{k, n_1, n_3, \dots, n_{2k+1}; n_{2k+1} \geq 1} 2^{n_1 + \dots + n_{2k+1}} \\
&\quad \frac{\left(\frac{1}{1!} \frac{i\nabla_\xi \cdot \nabla_x}{2} f(x)\right)^{n_1}}{n_1!} \frac{\left(\frac{1}{3!} \left(\frac{i\nabla_\xi \cdot \nabla_x}{2}\right)^3 f(x)\right)^{n_3}}{n_3!} \dots \frac{\left(\frac{1}{(2k+1)!} \left(\frac{i\nabla_\xi \cdot \nabla_x}{2}\right)^{2k+1} f(x)\right)^{n_{2k+1}}}{n_{2k+1}!} Q(\xi).
\end{aligned} \tag{A.2}$$

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