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L^2-EXPONENTIAL LOWER BOUNDS TO EXCITED STATES OF QUANTUM MECHANICAL SYSTEMS

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Abstract

Let $H = -\Delta + V$ be defined on $L^2(\mathbb{R}^n)$, $n \geq 3$. Let $V = V_1 + V_2$, $V_1 \in L^p(\mathbb{R}^n)$, for some $p > 2n/3$, $V_2 \in L^\infty(\mathbb{R}^n)$ and $|x|\partial V/\partial|x|$ relatively form bounded with respect to $-\Delta$ with relative bound < 2. It is proven that there exists an $\alpha_0 \geq 0$ such that $\forall\ \alpha \geq \alpha_0$, $e^{\alpha|x|}\psi(x) \notin L^2(\mathbb{R}^n)$, where ψ denotes an L^2-eigenfunction of H. Related results are also shown to hold for many body Schrödinger operators including atoms and molecules.

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I. Introduction and Results

In this paper we consider eigenfunctions of Schrödinger operators

$$H = -\Delta + V , \tag{1.1}$$

defined on $L^2(\mathbb{R}^n)$, $n \geq 3$, with V a real valued multiplication operator. We will deal with potentials which satisfy the following conditions:

(a) $$V = V_1 + V_2 \tag{1.2}$$

with

$$V_1 \in L^p(\mathbb{R}^n), \quad p = 2n/3 + \delta, \quad \delta > 0 , \tag{1.3}$$

$$V_2 \in L^\infty(\mathbb{R}^n). \tag{1.4}$$

(b) Let $x = (x_1, x_2, \ldots, x_n)$, $x_i \in \mathbb{R}$, $i = 1,2,\ldots,n$, $r = |x|$. Let $\Omega_{R_o} = \{x \in \mathbb{R}^n: r > R_o\}$ where R_o is arbitrarily large but finite. We require that for every $\phi \in C_o^\infty(\Omega_{R_o})$ the distributional derivative $r\partial V/\partial r$ satisfies

$$\int \phi^* |r\partial V/\partial r| \phi dx \leq a \, \|\nabla\phi\|^2 + b \, \|\phi\|^2 . \tag{1.5}$$

with $a < 2$, $b < \infty$. That is to say $r\partial V/\partial r$ is relatively form bounded with respect to $-\Delta$ with relative bound < 2.

Remark 1.1

Condition (a) implies that H is essentially selfadjoint on $C_o^\infty(\mathbb{R}^n)$ and that it is selfadjoint on the domain of the Laplacian, $D(-\Delta) = W^{2,2}(\mathbb{R}^n)$ [1], where $W^{2,2}$ denotes the usual Sobolev space [2]. Furthermore condition (a) implies via Theorem X.20 of reference [1] that V is relatively bounded with respect to $-\Delta$ with relative bound zero.

$$\|Vu\|^2 \leq \varepsilon \, \|\Delta u\|^2 + k(\varepsilon) \, \|u\|^2 \tag{1.6}$$

for all $u \in W^{2,2}(\mathbb{R}^n)$ and $\varepsilon > 0$ with

$$k(\varepsilon) \leq D\varepsilon^{-3(1-\gamma)} , \qquad \gamma = 6\delta/(n+6\delta) . \tag{1.7}$$

D is a suitable constant in which the L^∞-norm of V_2 has been absorbed. We notice that the proof of Theorem X.20 of ref. [1] extends to $n = 3$ for $p > 2$.

Our main result is the following

Theorem 1.1

Suppose ψ satisfies $H\psi = E\psi$, with E the corresponding real eigenvalue, H given by (1.1) and V satisfying the conditions (a) and (b). Then there exists an $\alpha_0 > 0$ such that for

$$\alpha \geq \alpha_0 , \qquad e^{\alpha|x|}\psi \notin L^2(\mathbb{R}^n) .$$

We shall state also an analogous result for n-body Schrödinger operators with 2-body potentials including the case of atomic and molecular Hamiltonians.

Let

$$L = - \sum_{i,j=1}^{N} a_{ij} \nabla_i \nabla_j \tag{1.8}$$

where ∇_i, ∇_j denote the 3-dimensional gradient operators and $a_{ij} \in \mathbb{R}$, $1 \leq i,j \leq N$. We assume that the matrix $A_N = (a_{ij})$ is positive definite. We consider the following eigenvalue problem

$$(L + W - E) \psi(x) = 0 \tag{1.9}$$

with $x_i \in \mathbb{R}^3$, $1 \leq i \leq N$, $x = (x^{(1)},x^{(2)},\dots,x^{(N)}) \in \mathbb{R}^{3N}$

$$W(x) = \sum_{i=1}^{N} V(x^{(i)}) + \sum_{i<j}^{N} V_{ij}(x^{(i)} - x^{(j)}) . \tag{1.10}$$

E denotes the eigenvalue with $\psi(x)$ the corresponding eigenfunction. Conditions (a) and (b) on the potential are now replaced by

(a') $V_i(y)$, $V_{ij}(y) \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for some $p > 2$, for all $1 \leq i,j \leq N$.

(b') Let $V(y)$ denote the multiplication operators V_i respectively V_{ij} on $\mathbb{R}^3$. We require that $|y|\partial V/\partial|y|$ (the distributional derivative) is relatively form bounded with respect to the 3-dimensional Laplacian with relative bound zero, that is to say for all $\varepsilon > 0$ there exists $C(\varepsilon) < \infty$ so that

$$\int |\phi|^2 |y| \partial V(y)/\partial |y| dy \leq \varepsilon \, ||\nabla\phi||^2 + C(\varepsilon) \, ||\phi||^2 \tag{1.11}$$

for all $\phi \in W^{1,2}(\mathbb{R}^3)$.

Theorem 1.2

Suppose ψ satisfies (1.9) and W obeys condition (a') and (b'). Then there exists an $\alpha_0 \geq 0$ such that for $\alpha \geq \alpha_0$, $e^{\alpha|x|}\psi \notin L^2(\mathbb{R}^{3N})$.

Remark 1.2

By removing the center of mass motion from a Hamiltonian describing an atom or a molecule consisting of N+1 particles one arrives at Hamiltonians as given in (1.9). The restriction to 3-dimensional particles is meaningless. Theorem 1.2 holds also in the case of Hamiltonians describing N-particle systems consisting of n-dimensional particles ($n \geq 3$).

Unfortunately Theorem 1.1 and Theorem 1.2 are not very strong. They simply tell us that an eigenfunction of a Hamiltonian as given in (1.1) and (1.9) decays in an averaged sense not faster than exponentially.

The situation is a lot more transparent for the case of upper bounds to subcontinuum wave functions and lower bounds to groundstates. For the atomic case upper bounds have been (to cite only the most recent results) derived by T. Hoffmann-Ostenhof et al. [3], Deift et al. [4] and Ahlrichs et al. [5]. The most general result is due to Agmon [6] who considers general many particle systems where condition (a) respectively (a') is replaced by $V \in L^p + (L^\infty)_\varepsilon$, $p > n/2$ which means that V can be split into two parts, V_1 and V_2 with $||V_2||_{L^\infty}$ arbitrarily small. Even exponentially decreasing upper bounds to eigenfunctions of pseudodifferential operators have been recently obtained by Sigal [7]. Lower bounds for groundstates of two electron atoms have been obtained by T. Hoffmann-Ostenhof [8] and in ref. [5] exhibiting the same exponential decay as the upper bounds.

Recently Carmona and Simon [9] showed that the Agmon result is in some sense optimal. The Agmon Carmona Simon results [6,9] tell us that any mathematical groundstate $\psi(x)$ (positive) of a Hamiltonian with potentials satisfying the conditions indicated above obeys $\lim_{|x|\to\infty} -[\ln \psi(x)]/\rho(x) = 1$, where $\rho(x)$ is an explicitly computable function depending on the spectral properties of the considered Hamiltonian. Lieb and Simon [10] (general many particle systems) and Combes et al. [11] (Helium groundstate) obtained even more detailed results for groundstates.

No such results are available for excited states, because excited states have nodes and the methods to obtain lower bounds (Maximum principle + Harnack inequality [5,7,12], path integral ideas [9]) do not work in these cases. There is even a class of potentials for which the Agmon Carmona Simon result holds for groundstates but for which in the case of excited states eigenfunctions of compact support have not been ruled out yet. However, for special cases the strong results of Mercuriev [13] (three-particle systems with short range potentials) and Bardos and Merigot [14] (one-particle systems) are available.

Our approach is somewhat related to the methods used recently by various authors to prove unique continuation theorems for elliptic partial differential operators [15-18]. In fact our L^p-condition (1.3) on V_1 is the same as the condition required by Saut and Scheurer [18].

To conclude this section we sketch the main ideas of the proof of Theorem 1.1. Theorem 1.2 follows from Theorem 1.1 quite easily.

First we note that any L^2-eigenfunction of (1.1) is uniformly continuous. This follows from the fact that for eigenfunctions of a Hamiltonian whose potential satisfies (a) Harnack-type inequalities hold [19,20] which imply continuity and for our case even Hölder continuity [19].

As a consequence we have

$$r\, e^{\alpha r}\psi \in W^{2,2}_{loc}(\mathbb{R}^n) \tag{1.12}$$

for differentiation introduces only $\frac{1}{r}$- terms. We shall assume that $r\, e^{\alpha r}\psi \in$ $\in W^{2,2}(\mathbb{R}^n)$ for arbitrarily large α and derive a contradiction.

The starting point for the proof is the identity

$$\|r\, e^{\alpha r}\Delta\psi\|^2 = \|r\, e^{\alpha r}(V-E)\psi\|^2 \quad . \qquad (1.13)$$

In section II we derive a lower bound to $\|r\, e^{\alpha r}\Delta f\|$ for $f \in W^{2,2}(\mathbb{R}^n) \cap C^0(\mathbb{R}^n)$ which may be interesting for itself - we do not claim originality since there is a rich literature on inequalities relating weighted Sobolev spaces. Combining this bound with an upper bound to the r.h.s. of (1.13) leads to a lower bound to $\|r\, e^{\alpha r}\psi\|^2$ with an $\exp(\alpha^{(1+\delta)})$ behaviour for large α, and some $\delta > 0$.

In section III the basic identity is

$$\int e^{2\alpha r}\chi r^2\psi^*(H-E)r\,\frac{\partial\psi}{\partial r}\,dx = \int e^{2\alpha r} r^2\chi\psi^*(r\,\frac{\partial V}{\partial r} + 2(V-E))\psi dx \qquad (1.14)$$

where χ is some positive $C^\infty(\mathbb{R}^n)$ function with support in Ω_{R_0}. From (1.14) we derive an upper bound to $\|\sqrt{\chi}\, r\, e^{\alpha r}\psi\|$ which behaves for large α like $e^{\alpha c}$ for some $c > 0$. In section IV we complete the proof of Theorem 1.1 and show how Theorem 1.2 follows via Theorem 1.1.

II. A Lower Bound to $\|r\, e^{\alpha r}\psi\|$

We start with the following

Lemma 2.1

Let f be continuous and $f \in W^{2,2}(\mathbb{R}^n)$. Suppose $e^{\alpha r}\, r\, \Delta f \in L^2(\mathbb{R}^n)$ and $e^{\alpha r}\sqrt{r}\, f \in L^2(\mathbb{R}^n)$, then

$$\|r\, e^{\alpha r}\Delta f\|^2 \geq 4\alpha^3\|r^{1/2}\, e^{\alpha r} f\|^2 + 2\alpha^2\|e^{\alpha r} f\|^2 \quad . \qquad (2.1)$$

Proof of Lemma 2.1

Suppose first that $f \in C^\infty(\mathbb{R}^n)$ and that the integrals in (2.1) exist. We consider f in spherical coordinates $f = f(r\zeta)$, $\zeta = x/r$. Following Schechter and Simon [15] we expand f

$$r^{\frac{n-1}{2}} f(r\zeta) = \sum_{\ell,m} f_{\ell,m}(r)\, Y_{\ell,m}(\zeta)$$

where the $\{Y_{\ell,m}\}$ are surface harmonics which form a complete orthogonal set in $L^2(S^{n-1})$ with S^{n-1} the unit sphere $|x| = 1$ in $\mathbb{R}^n$. The $f_{\ell,m}(r)$ are given by

$$f_{\ell,m}(r) = r^{\frac{n-1}{2}} \int_{S^{n-1}} f(r\zeta)\, Y^*_{\ell,m}(\zeta) d\zeta \; .$$

Denoting

$$L_s f(r) := f'' - s(s+1)r^{-2} f \; , \qquad s = \frac{1}{2}(2\ell + n - 3)$$

where the prime denotes differentiation with respect to r we have

$$\Delta f(r\zeta) = r^{-\frac{n-1}{2}} \sum_{\ell,m} L_s\, f_{\ell,m}(r)\, Y_{\ell,m}(\zeta) \; .$$

Using the orthonormality of the surface harmonics we obtain

$$\|r\, e^{\alpha r} \Delta f\|^2 = \sum_{\ell,m} \int |L_s f_{\ell,m}|^2 e^{2\alpha r} r^2 dr =$$

$$= \sum_{\ell,m} \{\int |f''_{\ell,m}|^2 r^2 e^{2\alpha r} dr + s^2(s+1)^2 \int |f_{\ell,m}|^2 r^{-2} e^{2\alpha r} dr$$

$$- 2 \,\mathrm{Re}\, s(s+1) \int f^*_{\ell,m} f''_{\ell,m} e^{2\alpha r} dr\} \; .$$

Partial integration leads to

$$\|r\, e^{\alpha r} \Delta f\|^2 = \sum_{\ell,m} \int \{ |f''_{\ell,m}|^2 r^2 e^{2\alpha r} dr + 2s(s+1) \int |f'_{\ell,m}|^2 e^{2\alpha r} dr$$

$$- 4s(s+1)\alpha^2 \int |f_{\ell,m}|^2 e^{2\alpha r} dr + s^2(s+1)^2 \int |f_{\ell,m}|^2 e^{2\alpha r} r^{-2} dr\} \; , \qquad (2.2)$$

By the Cauchy-Schwarz inequality

$$\int |f'_{\ell,m}|^2 e^{2\alpha r} dr \geq \alpha^2 \int |f_{\ell,m}|^2 e^{2\alpha r} dr \qquad (2.3)$$

and by applying Cauchy-Schwarz twice we get

$$\int|f''_{\ell,m}|^2e^{2\alpha r}r^2dr \geq \alpha^4 \int|f_{\ell,m}|^2r^2e^{2\alpha r}dr + 4\alpha^3 \int|f_{\ell,m}|^2r\, e^{2\alpha r}dr$$

$$+ \alpha^2 \int|f_{\ell,m}|^2e^{2\alpha r}dr \ . \qquad (2.4)$$

Combining (2.2) with (2.3) and (2.4) we get

$$\|r\, e^{\alpha r}\Delta f\|^2 \geq \sum_{\ell,m} \{\int(\alpha^2-s(s+1)r^{-2})^2r^2e^{2\alpha r}|f_{\ell,m}|^2dr$$

$$+ 4\alpha^3 \int r\, e^{2\alpha r}|f_{\ell,m}|^2dr + 2\alpha^2 \int e^{2\alpha r}|f_{\ell,m}|^2dr\} \geq$$

$$\geq 4\alpha^3 \|r^{1/2}\, e^{\alpha r}f\|^2 + 2\alpha^2 \|e^{\alpha r}f\|^2 \ .$$

Hence (2.1) holds for $f \in C^\infty(\mathbb{R}^n)$ provided the occurring integrals exist.

Now we have to show that inequality (2.1) holds also for $f \in W^{2,2}(\mathbb{R}^n) \cap$ $\cap\, C^0(\mathbb{R}^n)$. For this we regularize f. Let $J(x) \in C_0^\infty(\mathbb{R}^n)$, $J(x) \geq 0$, $J(x) = 0$ for $|x| \geq 1$ and $\int J(x)dx = 1$. For $\varepsilon > 0$ let $J_\varepsilon(x) = \varepsilon^{-n} J(x/\varepsilon)$ and for $u \in L^1_{loc}(\mathbb{R}^n)$ let $u_\varepsilon := \int J_\varepsilon(x-y)u(y)dy = J_\varepsilon * u$. We have $u_\varepsilon \in C^\infty(\mathbb{R}^n)$. Suppose $e^{\alpha r}r^m u \in L^2(\mathbb{R}^n)$ for some $m \geq 0$ and $\alpha \geq 0$. Then, by Cauchy-Schwarz's inequality

$$|u_\varepsilon(x)|^2 \leq \int_{\mathbb{R}^n} J_\varepsilon(x-y)|u(y)|^2dy$$

and further we get

$$\int_{\mathbb{R}^n} e^{2\alpha r}r^{2m}|u_\varepsilon(x)|^2dx \leq \int_{\mathbb{R}^n}\int_{|z|\leq 1} e^{2\alpha r}r^{2m}\, J(z)|u(x-\varepsilon z)|^2dxdz \leq$$

$$\leq \sup_{|z|\leq 1} \int_{\mathbb{R}^n} e^{2\alpha r}\, r^{2m}|u(x-\varepsilon z)|^2dx \leq$$

$$\leq \sup_{|z|\leq 1} \int_{\mathbb{R}^n} e^{2\alpha(|y|+\varepsilon|z|)}(|y|+\varepsilon|z|)^{2m}|u(y)|^2dy \leq$$

$$\leq e^{2\alpha\varepsilon}[\int e^{2\alpha r}r^{2m}|u(x)|^2dx + (1-\delta_{mo}) \sum_{k=1}^{2m} \binom{2m}{k} \varepsilon^k \int e^{2\alpha r}r^{2m-k}|u(x)|^2dx] \ . \qquad (2.5)$$

This implies

$$\limsup_{\varepsilon\to 0} \int e^{2\alpha r} r^{2m} |u_\varepsilon|^2 dx \le \int e^{2\alpha r} r^{2m} |u(x)|^2 dx \,. \tag{2.6}$$

Since $f \in C^0(\mathbb{R}^n)$ we have

$$\lim_{\varepsilon\to 0} e^{2\alpha r}\, r^{2m} |f_\varepsilon(x)|^2 = e^{2\alpha r}\, r^{2m}\, |f(x)|^2$$

pointwise and by Fatou's lemma

$$\int e^{2\alpha r}\, r^{2m}\, |f(x)|^2 dx = \int \liminf_{\varepsilon\to 0} e^{2\alpha r}\, r^{2m} |f_\varepsilon(x)|^2 dx \le$$

$$\le \liminf_{\varepsilon\to 0} \int e^{2\alpha r}\, r^{2m}\, |f_\varepsilon(x)|^2 dx \,. \tag{2.7}$$

Hence (2.6) with $u = f$ and (2.7) imply

$$\lim_{\varepsilon\to 0} \int e^{2\alpha r}\, r^{2m}\, |f_\varepsilon|^2 dx = \int e^{2\alpha r}\, r^{2m}\, |f|^2 dx \,. \tag{2.8}$$

Now we choose $u = \Delta f$ and $m = 1$ in (2.5). Since $f \in W^{2,2}(\mathbb{R}^n)$, $\Delta f_\varepsilon(x) =$ $= (\Delta f)_\varepsilon(x)$ and

$$\limsup_{\varepsilon\to 0} \int e^{2\alpha r}\, r^2 |\Delta f_\varepsilon|^2 dx \le \int e^{2\alpha r}\, r^2 |\Delta f|^2 dx \,. \tag{2.9}$$

The L^2-conditions on f and Δf imply with (2.5) that (2.1) holds for f_ε. (2.8) with $m = 0$ respectively $1/2$ and (2.9) imply that if we replace f by f_ε in (2.1) and take the limit $\varepsilon \to 0$ on both sides that (2.1) holds also for f. □

Remark 2.1

We also tried to obtain related inequalities for $\| r^{\gamma/2} e^{\alpha r} \Delta f \|$, but only for $\gamma = 2$ our procedure was successful. Lemma 2.1 appears to be related to a family of inequalities of Hörmander [21] which have been used for instance by Georgescu [16] and Saut and Scheurer [18] to prove unique continuation. Note however the different powers of r occurring on both sides of (2.1).

Next we shall derive an upper bound to $\|r\, e^{\alpha r}\Delta\psi\|$ from which together with Lemma 2.1 the desired lower bound to $\|r\, e^{\alpha r}\psi\|$ will follow.

Lemma 2.2

Let $H\psi = E\psi$, with H given by (1.1) and V obeying condition (a). Suppose $e^{\alpha r} r\psi \in W^{2,2}(\mathbb{R}^n)$ for finite $\alpha \geq 0$. Then for sufficiently large α and $1 > \varepsilon > 0$

$$\|e^{\alpha r} r\Delta\psi\|^2 \leq C\{(\varepsilon\alpha^4 + k(\varepsilon))\, \|r\, e^{\alpha r}\psi\|^2 + \varepsilon\alpha^3\, \|r^{1/2}\, e^{\alpha r}\psi\|^2 + + \varepsilon\alpha^2\, \|e^{\alpha r}\psi\|^2\} \tag{2.10}$$

with $k(\varepsilon)$ given as in (1.7) and C a suitable constant.

Proof of Lemma 2.2

Since $W \equiv V - E$ obeys condition (a) we have by Remark 1.1 for $\varepsilon > 0$

$$\|e^{\alpha r} r\Delta\psi\|^2 = \|W\, e^{\alpha r} r\psi\|^2 \leq \varepsilon\, \|\Delta e^{\alpha r} r\psi\|^2 + k(\varepsilon)\, \|e^{\alpha r} r\psi\|^2 \; . \tag{2.11}$$

Obviously

$$\|\Delta e^{\alpha r} r\psi\|^2 \leq 3\,[\, \|e^{\alpha r} r\Delta\psi\|^2 + 4\, \|(\nabla\psi)(\nabla e^{\alpha r} r\psi)\|^2 + \|\psi\Delta e^{\alpha r} r\|^2\,] \tag{2.12}$$

and we proceed by estimating the second term on the r.h.s, of (2.12). For a sufficiently well behaved real valued function f we get by partial integration

$$\|f\nabla\psi\|^2 = \|\nabla f\psi\|^2 + \int |\psi|^2 f\Delta f dx \; . \tag{2.13}$$

Since ψ is an eigenfunction of H it is easily seen that

$$\|\nabla f\psi\|^2 + \int W|f\psi|^2 dx = \|\psi\nabla f\|^2 \; . \tag{2.14}$$

The ε-boundedness of W with respect to $-\Delta$ also implies ε-formboundedness with respect to $-\Delta$. That means for any $\delta > 0$ there is a constant $C(\delta)$ such that for $f\psi \in W^{1,2}(\mathbb{R}^n)$

$$\| \, |W|^{1/2} f\psi \|^2 \leq \delta \, \|\nabla f\psi\|^2 + C(\delta) \, \|f\psi\|^2 \; . \tag{2.15}$$

(2.14) and (2.15) lead to

$$\|\nabla f\psi\|^2 \leq \frac{1}{1-\delta} \left(\|\psi\nabla f\|^2 + C(\delta) \, \|f\psi\|^2 \right) \tag{2.16}$$

for $\delta < 1$ and we get with (2.13)

$$\|f\nabla\psi\|^2 \leq \frac{1}{1-\delta} \left(\|\psi\nabla f\|^2 + C(\delta) \, \|f\psi\|^2 \right) + \int |\psi|^2 f\Delta f dx \; . \tag{2.17}$$

Identifying f with $\frac{\partial}{\partial r}(r\, e^{\alpha r}) = (1 + \alpha r)e^{\alpha r}$ we have

$$\|(\nabla\psi)(\nabla r\, e^{\alpha r})\|^2 \leq \| \, |\nabla\psi| \, |\nabla r\, e^{\alpha r}| \, \|^2 \leq$$

$$\leq \frac{1}{1-\delta} \left[\|\psi e^{\alpha r}(2\alpha + r\alpha^2)\|^2 + C(\delta) \, \|e^{\alpha r}\psi\|^2 \right] +$$

$$+ \alpha^2 \int |\psi|^2 e^{2\alpha r} \left\{ \frac{2n-2}{r} + 3n\alpha + (n+3)\alpha^2 r^2 + \alpha^3 r^2 \right\} dx \; . \tag{2.18}$$

Working out $\|\psi\Delta e^{\alpha r} r\|$ and combining the inequalities (2.11), (2.12) and (2.18) we arrive at

$$(1-\varepsilon) \, \|e^{\alpha r} r\Delta\psi\|^2 \leq C_1 \{ \varepsilon \int |\psi|^2 e^{2\alpha r} (\alpha^4 r^2 + \alpha^3 r + \alpha^2 + 1 + \alpha r^{-1} + r^{-2}) dx$$

$$+ k(\varepsilon) \, \|e^{\alpha r} r\psi\|^2 \} \; . \tag{2.19}$$

Thereby the δ-dependence has been absorbed into C_1 and since we are interested in large α we estimated every power of r by that term which contains the largest power of α.

To bound the r^{-1} and r^{-2} terms in (2.19) we use (2.16) and get

$$\|\nabla e^{\alpha r}\psi\|^2 \leq \frac{C(\delta) + \alpha^2}{1-\delta} \, \|e^{\alpha r}\psi\|^2 \; . \tag{2.20}$$

Cauchy-Schwarz implies the well-known estimate

$$\|\nabla e^{\alpha r}\psi\|^2 \geq \|\frac{\partial}{\partial r}(e^{\alpha r}\psi)\|^2 \geq \frac{(n-2)^2}{4}\|r^{-1} e^{\alpha r}\psi\|^2$$

and hence

$$\|r^{-1} e^{\alpha r}\psi\|^2 \leq C_2\alpha^2 \|e^{\alpha r}\psi\|^2 \tag{2.21}$$

for sufficiently large α and suitable C_2. Analogously using the well-known estimate

$$\|\nabla e^{\alpha r}\psi\| \geq \frac{n-1}{2}\frac{\|r^{-1} e^{\alpha r}\psi\|^2}{\|e^{\alpha r}\psi\|}$$

we obtain

$$\|r^{-1/2} e^{\alpha r}\psi\|^2 \leq C_3\alpha \|e^{\alpha r}\psi\|^2 \tag{2.22}$$

for sufficiently large α and suitable C_3.

Inserting (2.21) and (2.22) in (2.19) yields (2.10) for $\varepsilon < 1$. □

Finally we shall obtain the desired lower bound:

Lemma 2.3

Suppose ψ satisfies the conditions of Lemma 2.2, then for α sufficiently large

$$\|r e^{\alpha r}\psi\|^2 \geq m_1 \|r^{1/2} e^{\alpha r}\psi\| \alpha^\sigma \geq m_2 \alpha^\sigma e^{\alpha^{(1+\sigma)}} \tag{2.23}$$

where m_1 and m_2 are suitable positive constants and $\sigma > 0$ depends on the δ in (1.3).

Proof of Lemma 2.3

As we already noted in the introduction $\psi \in W^{2,2}(\mathbb{R}^n) \cap C^0(\mathbb{R}^n)$. Hence by Lemma 2.1 and 2.2 we see that

$$4\alpha\,\|r^{1/2}e^{\alpha r}\psi\|^2 + 2\,\|e^{\alpha r}\psi\|^2 \le C[(\varepsilon\alpha^2 + \frac{k(\varepsilon)}{\alpha^2})\|r\,e^{\alpha r}\psi\|^2 + \varepsilon\alpha\,\|r^{1/2}e^{\alpha r}\psi\|^2 + \varepsilon\,\|e^{\alpha r}\psi\|^2]\ . \tag{2.24}$$

By (1.7), $k(\varepsilon) \le D'\varepsilon^{-3(1-\gamma)}$ for suitable D'. Hence we get for sufficiently small ε

$$\|r^{1/2}e^{\alpha r}\psi\|^2 \le \frac{C}{4-C\varepsilon}(\varepsilon\alpha + D'\varepsilon^{-3(1-\gamma)}\alpha^{-3})\,\|r\,e^{\alpha r}\psi\|^2\ .$$

Choosing $\varepsilon = \alpha^{-(1+\sigma)}$ with $0 < \sigma \le \frac{3\gamma}{4-3\gamma}$ we obtain

$$\|r^{1/2}\,e^{\alpha r}\psi\|^2 \le M\alpha^{-\sigma}\,\|r\,e^{\alpha r}\psi\|^2 \tag{2.25}$$

for $\alpha \ge \alpha_0$, α_0 sufficiently large and suitable M. We regard $\|r^{1/2}e^{\alpha r}\psi\|^2$ as a function of α and denote it by $J(\alpha)$. Then (2.25) can be written as

$$\frac{J'(\alpha)}{J(\alpha)} \ge \frac{2}{M}\,\alpha^{\sigma}\ . \tag{2.26}$$

Integration of this differential inequality from α_0 to α gives

$$J(\alpha) \ge d\ e^{\alpha^{(1+\sigma)}}$$

for $\alpha \ge \alpha_0$ and suitable d, from which together with (2.25) inequality (2.23) follows. □

III. The Upper Bound to $\|r\,e^{\alpha r}\psi\|$

Let $\chi \in C^\infty(\mathbb{R}^n)$, χ radially symmetric, $\chi \ge 0$, $\frac{\partial\chi}{\partial r} \ge 0$, supp $\chi \subset \Omega_{R_0}$ and $\chi = 1$ for $r \ge R_1 > R_0$. Here R_0 and Ω_{R_0} is as in condition (b).

Lemma 3.1

Let ψ satisfy the Schrödinger equation $H\psi = E\psi$ with H given by (1.1) and suppose V satisfies condition (a) and (b). Suppose $r\,e^{\alpha r}\psi \in W^{2,2}(\mathbb{R}^n)$

for finite α, then for a suitable constant C and sufficiently large α

$$\|r\, e^{\alpha r}\, \chi^{1/2}\, \psi\|^2 \leq C\, e^{2\alpha R_1} . \tag{3.1}$$

Proof of Lemma 3.1

First we consider (1.11) and derive it formally. We have

$$(H - E)x_i\psi = -2\frac{\partial\psi}{\partial x_i}, \qquad i = 1,2,\dots,n .$$

Partial differentiation leads to

$$\frac{\partial}{\partial x_i}(H-E)x_i\psi = (H-E)x_i\frac{\partial\psi}{\partial x_i} + \frac{\partial V}{\partial x_i}x_i\psi = -\frac{\partial^2\psi}{\partial x_i^2}$$

and since $\sum x_i \frac{\partial}{\partial x_i} = x\nabla = r\frac{\partial}{\partial r}$,

$$(H-E)r\frac{\partial\psi}{\partial r} = -2\Delta\psi - r\frac{\partial V}{\partial r}\psi . \tag{3.2}$$

It is easy to see that (3.2) holds in the quadratic form sense since by assumption $r\psi \in W^{2,2}(\mathbb{R}^n) \cap C^0(\mathbb{R}^n)$, $r\frac{\partial\psi}{\partial r} \in W^{1,2}(\mathbb{R}^n)$ the form domain of H.

We shall also use the following relation

$$(H-E)f\psi = -\psi\Delta f - 2\nabla f\nabla\psi \tag{3.3}$$

which holds in the form sense for sufficiently well behaved f. Choosing $f = r^2\chi e^{2\alpha r}$ we have

$$-\int(x\nabla\psi^*)(H-E)e^{2\alpha r}r^2\chi dx = 4\int\left|\frac{\partial\psi}{\partial r}\right|^2 e^{2\alpha r}(\alpha r^3+r^2)\chi dx +$$

$$+ 2\int\psi\frac{\partial\psi^*}{\partial r}e^{2\alpha r}\chi[2\alpha^2r^3 + (3+n)\alpha r^2 + nr]dx + F_1(\alpha) , \tag{3.4}$$

Thereby F_1 and later on F_2, F_3, F_4 will denote sums of integrals with integrands containing derivatives of χ. Partial integration together with (3.2) and (3.4) leads to

$$\int e^{2\alpha r} r^2 \chi |\psi|^2 (2(V-E) + r \frac{\partial V}{\partial r}) dx = \int r \frac{\partial \psi^*}{\partial r} (H-E) e^{2\alpha r} r^2 \chi \psi dx =$$

$$= 2\{\int |\frac{\partial \psi}{\partial r}|^2 e^{2\alpha r} (2\alpha r^3 + 2r^2) \chi dx - 2\alpha^3 \int r^3 e^{2\alpha r} |\psi|^2 \chi dx - \tag{3.5}$$

$$- (5+2n)\alpha^2 \int r^2 e^{2\alpha r} \chi |\psi|^2 dx - \frac{n^2+6n+3}{2} \alpha \int r |\psi|^2 e^{2\alpha r} \chi dx - \frac{n^2}{2} \int |\psi|^2 e^{2\alpha r} \chi dx\} + F_2 .$$

Now by Cauchy-Schwarz's inequality and partial integration

$$\int_0^\infty |\frac{\partial \psi}{\partial r}|^2 e^{2\alpha r} r^m \chi dr \geq [\mathrm{Re} \int_0^\infty \psi \frac{\partial \psi^*}{\partial r} e^{2\alpha r} r^m \chi dr]^2 (\int_0^\infty |\psi|^2 e^{2\alpha r} r^m \chi dr)^{-1} \tag{3.6}$$

where we used $\chi \geq 0$, $\frac{\partial \chi}{\partial r} \geq 0$. For $m = n+2$, $n+1$ (3.6) combined with (3.5) leads to

$$\int e^{2\alpha r} r^2 \chi |\psi|^2 (V-E + \frac{1}{2} r \frac{\partial V}{\partial r}) dx \geq$$

$$\geq \alpha^2 \int r^2 e^{2\alpha r} \chi |\psi|^2 dx - \frac{1}{2}(n^2 - 1 + 2n)\alpha \int r \, e^{2\alpha r} \chi |\psi|^2 dx -$$

$$- \frac{n^2}{2} \int e^{2\alpha r} \, e^{2\alpha r} \chi |\psi|^2 dx + F_2 . \tag{3.7}$$

Since V obeys condition (a) it is ε-formbounded with respect to $- \Delta$, so for all $\varepsilon > 0$

$$||e^{\alpha r} \sqrt{\chi} \, r \, \psi |V-E|^{1/2}||^2 \leq \varepsilon \, ||\nabla \sqrt{\chi} \, r \, e^{\alpha r} \psi||^2 + C(\varepsilon) \, ||\sqrt{\chi} \, r \, e^{\alpha r} \psi||^2 . \tag{3.8}$$

By condition (b) we have

$$||e^{\alpha r} \sqrt{\chi} \, r \psi |r \frac{\partial V}{\partial r}|^{1/2} ||^2 \leq a \, ||\nabla \sqrt{\chi} \, r \, e^{\alpha r} \psi||^2 + b \, ||\sqrt{\chi} \, r \, e^{\alpha r} \psi||^2 \tag{3.9}$$

with $a < 2$ by (1.5). In order to bound $||\nabla \sqrt{\chi} \, r \, e^{\alpha r} \psi||$ from above we use inequality (2.16) and obtain for $0 < \delta < 1$

$$||\nabla \sqrt{\chi} \, e^{\alpha r} r \, \psi||^2 \leq \frac{1}{1-\delta} [(\alpha^2 + C(\delta)) \, ||\sqrt{\chi} \, r \, e^{\alpha r} \psi||^2 + 2\alpha \, ||\sqrt{r\chi} \, e^{\alpha r} \psi||^2 +$$

$$+ ||\sqrt{\chi} \, e^{\alpha r} \psi||^2 + F_3] . \tag{3.10}$$

For ε and δ sufficiently small (3.8), (3.9) and (3.10) imply the following upper bound to the l.h.s. of (3.7)

$$\int e^{2\alpha r} r^2 \chi |\psi|^2 |V - E + \frac{1}{2}\, \iota\, \frac{\partial V}{\partial r}| dx \leq (C_1\alpha^2 + C_2)\, \|\sqrt{\chi}\, e^{\alpha r} r\psi\|^2 +$$

$$+ C_1 [2\alpha\, \|\sqrt{r\chi}\, e^{\alpha r}\psi\|^2 + \|\sqrt{\chi}\, e^{\alpha r}\psi\|^2 + F_3] \qquad (3.11)$$

for suitable $0 < C_1 < 1$, $C_2 > 0$. Next we combine (3.7) with (3.11) and take into account that supp χ Ω_{r_0} with R_o arbitrarily large. Then it is easily seen that for sufficiently large α

$$\alpha^2\, \|\sqrt{\chi}\, e^{\alpha r} r\psi\|^2 \leq F_4(\alpha)\ . \qquad (3.12)$$

Since all integrals occurring in F_4 contain derivatives of χ which have support in $\{x \in \mathbb{R}^n:\ R_o \leq |x| \leq R_1\}$ it follows by L^∞-estimates that for some suitable k (not depending on α)

$$F_4(\alpha) \leq k\, e^{2\alpha R_1} \qquad \text{for } \alpha \geq 1\ .$$

This together with (3.12) proves inequality (3.1). □

IV. Proof of Theorem 1.1 and Theorem 1.2

First we complete the proof of Theorem 1.1; Since $1-\chi$ has compact support we conclude by Lemma 2.3 that for suitable $d > 0$, $\tau > 0$

$$\|\sqrt{\chi}\, e^{\alpha r} r\psi\|^2 = \|r\, e^{\alpha r}\psi\|^2 - \|\sqrt{1-\chi}\, r\, e^{\alpha r}\psi\|^2 \geq d e^{\alpha^{1+\tau}}$$

for sufficiently large α. But this is a contradiction to Lemma 3.1 for sufficiently large α. Hence $\sqrt{\chi}\, r\, e^{\alpha r}\psi \notin W^{2,2}(\mathbb{R}^n)$ for $\alpha > \bar{\alpha}$, $\bar{\alpha}$ sufficiently large, and consequently $r\, e^{\alpha r}\psi \notin W^{2,2}(\mathbb{R}^n)$ for $\alpha \geq \bar{\alpha}$, Using (2.12) and (2.16) it is easy to see that

$$\|e^{\alpha r} r\psi\|_{W^{2,2}(\mathbb{R}^n)} = \|e^{\alpha r} r\psi\| + \|\nabla e^{\alpha r} r\psi\| + \|\Delta e^{\alpha r}\psi\| \leq$$

$$\leq C(\|e^{\alpha r} r\psi\| + \|e^{\alpha r} \sqrt{r}\, \psi\| + \|e^{\alpha r}\psi\|)$$

where $C = C(\alpha)$ is bounded for finite α. Since the l.h.s. of this inequality is monotonically increasing in α and diverges for $\alpha \to \bar{\alpha}$, $e^{\alpha r}\psi \notin L^2(\mathbb{R}^n)$ for $\alpha \geq \alpha_0$ for suitable α_0. □

Remark 4.1

We note that in the proof of Theorem 1.1 we actually needed (1.6), (1.7), a consequence of condition (a), rather than condition (a) itself.

Remark 4.2

Our proof of Theorem 1.1 differs in several steps from the proofs of unique continuation theorems [15-18]. There usually a contradiction is already achieved by considering upper and lower bounds to $\|f\Delta\psi\|$ for suitably chosen f We could not achieve such a contradiction because of the different powers of r in Lemma 2.1, and the subsequent estimates in Lemma 2.2, namely (2.10). However, if we replace conditions (a) and (b) by the requirements that $V \in L^p(\mathbb{R}^n)$ for some $p > \max(2, n/2)$ and rV^2 is relatively formbounded with respect to $-\Delta$, then it is also not difficult to show that $e^{\alpha r}\psi \notin L^2(\mathbb{R}^n)$ for sufficiently large α.

We sketch now the proof of Theorem 1.2. Denoting

$$x = (x^{(1)}, \ldots, x^{(N)}) \equiv (x_1, x_2, \ldots, x_{3N}) , \quad x_i \in \mathbb{R}$$

equation (1.9) can be written as

$$(-\sum_{i,j=1}^{3N} A_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + W - E)\, \psi(x) = 0 \qquad (4.1)$$

with $A \equiv A_N \otimes I_3$ symmetric and positive definite. Let P denote an orthogonal matrix with $P^T A P = (\lambda_i \delta_{ij})$ and let $D = (\lambda_i^{-1/2} \delta_{ij})$. Then the non singular transformation $y = xQ$ with $Q = PD$ transforms equation (4.1) into

$$[-\Delta + \tilde{W}(y) - E]\,\tilde{\psi}(y) = 0 \qquad (4.2)$$

where $\psi(x) \to \tilde{\psi}(y)$, $W(x) \to \tilde{W}(y)$ under the transformation. Obviously it suffices to show that $\tilde{W}(y)$ satisfies condition (a) (or rather (1.6), (1.7)) and (b). Then Theorem 1.1 implies that $e^{\alpha|y|}\tilde{\psi}(y) \notin L^2(\mathbb{R}^{3N})$, for sufficiently large α.

Since V_i, V_{ij} $(1 \le i,j \le N)$ obey condition (a') we conclude following Theorem X.20 of ref. [1] that V_{ij}, V_i obey (1.6) and (1.7) in $\mathbb{R}^3$. Again following arguments of ref. [1] (p. 166) it is easily shown that $W(x)$ satisfies (1.6) and (1.7). Since (A_{ij}) is positive definite standard arguments (Fourier transforms) show that $W(x)$ is ε-bounded with respect to $-\Delta$ on $\mathbb{R}^{3N}$ with $k(\varepsilon)$ as in (1.7). In a similar way it is easily seen that condition (b') implies ε-formboundedness of $|y|\partial\tilde{W}(y)/\partial|y|$ relative to $-\Delta$ on $\mathbb{R}^{3N}$. □

<u>Remark 4.3</u>

Actually condition (b') can be weakened. ε-formboundedness of $|y|\partial V(y)/\partial|y|$ can be replaced by the requirement that $|y|\partial V(y)/\partial|y|$ is formbounded with relative bound C where C depends on the number of particles.

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