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Pointwise Bounds on Eigenfunctions and Wave Packets in N-Body Quantum Systems IV*

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Abstract. We describe several new techniques for obtaining detailed information on the exponential falloff of discrete eigenfunctions of N-body Schrödinger operators. An example of a new result is the bound (conjectured by Morgan) $|\psi(x_1 \dots x_N)| \leqq C \exp(-\sum_1^N \alpha_n r_n)$ for an eigenfunction ψ of

$$H_N = -\sum_{i=1}^{N} \left(\Delta_i - \frac{Z}{|x_i|}\right) + \sum_{i<j} |x_i - x_j|^{-1}$$

with energy E_N. In this bound $r_1 r_2 \dots r_N$ are the radii $|x_i|$ in increasing order and the α's are restricted by $\alpha_n < (E_{n-1} - E_n)^{1/2}$, where E_n, for $n = 0, 1, \dots, N-1$, is the lowest energy of the system described by H_n. Our methods include subharmonic comparison theorems and "geometric spectral analysis".

§ 1. Introduction

It is an elementary fact that a solution of $(-\Delta + V)\psi = E\psi$ with $\psi \in L^2$, $V \to 0$ at ∞ (in some sense) and $E < 0$ has exponential falloff: it is certainly bounded (in some sense) by $C(\exp(-(1-\varepsilon)\sqrt{-E}|x|)$ for any $\varepsilon > 0$. Our interest here is in a considerably more subtle situation. Let

$$\tilde{H} = -\sum_{i=1}^{N} (2m_i)^{-1} \Delta^i + \sum_{i<j}^{1 \dots N} V_{ij}(x^i - x^j) \tag{1.1}$$

on $L^2(R^{\nu N})$ be the Schrödinger operator for N particles with coordinates $x^i \in R^\nu$, where Δ^i = Laplacian with respect to x^i. The operator H obtained by separating the center of mass motion acts on $L^2(X)$ where X is the $\nu(N-1)$-dimensional subspace $\Sigma m_i x^i = 0$ of $R^{\nu N}$. (Kinematics is discussed in Appendix 1). We consider solutions of

$$H\psi = E\psi. \tag{1.2}$$

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While $H = -\Delta + V$ in a suitable metric on X, it is no longer true that $V \to 0$ at infinity, even if each $V_{ij}(y) \to 0$ as $y \to \infty$ in R^ν, since V is not small in directions where $x \to \infty$ but some $|x^i - x^j|$ stays bounded. Thus the falloff of solutions of (1.2) is in general much slower than in the elementary case $V \to 0$ at ∞ and will depend sensitively on the direction in which $x \to \infty$.

There is extensive discussion of this problem in the chemical, physical and mathematical literature. The first result for general N-body systems (with $N > 3$) was obtained by O'Connor [23] (Some of the earlier literature is quoted in [25]; we mention here the work of Slaggie and Wichmann [30] on the case $N = 3$, and Alrich's [2] work on the N-electron atomic case.) O'Connors result is that

$$\int_X dx |\psi(x)|^2 e^{2\alpha|x|} < \infty \tag{1.3}$$

so long as

$$\alpha < (\Sigma - E)^{1/2}, \tag{1.4}$$

where Σ is the bottom of the continuous spectrum of H and $|x|$ the norm in configuration space defined by (A 1.1). Substantial simplifications of O'Connors proof and an extension to bound states embedded in the continuum were obtained by Combes and Thomas [9]. Starting from (1.3) Simon [26] derived the pointwise bound

$$|\psi(x)| \leqq C_\alpha \exp(-\alpha|x|). \tag{1.5}$$

for the same range of α. We will refer to (1.3)–(1.5) as COST estimates.

O'Connor [23] stated that his estimates were "best possible" by giving examples where the range of α could not be increased. Indeed we expect that if one restricts oneself to *isotropic bounds* (i.e. depending only on $|x|$), then (1.5) cannot be improved except by allowing $\alpha = (\Sigma - E)^{1/2}$ with perhaps a factor $|x|^\beta$ in front of the exponential ($\beta < 0$ is possible). This kind of improvement is obtained for the electron density in an atom by M. and T. Hoffmann-Ostenhof [15].

Our own attitude towards the problem was changed by a paper of Morgan [22] who pointed out that in directions where all $|x^i - x^j|$ go to infinity, ψ asymptotically satisfies $-\Delta\psi = E\psi$, so that one expects a falloff like $\psi \sim \exp(-\Sigma\alpha_i x^i)$ with $\sum \alpha_i^2/2m_i = E$, which may be considerably more rapid than (1.5). Morgan also showed how to use the Slaggie-Wichmann methods to improve (1.5) in the case $N = 3$. (It should be mentioned that there is a paper by Mercuriev [21] with stronger results on 3-particle systems, of which we were unaware, and that when M. and T. Hoffmann-Ostenhof first raised the issue of improving (1.5), it was one of us (B.S.) who assured them that (1.5) was "best possible"!)

Our goal in this paper is to develop general methods which can detect anisotropic exponential falloff properties of ψ. Two main themes are involved: the more "elementary" (§ 2) takes off from Morgan's remark and uses a subharmonic comparison theorem of the type already applied in III of this series [27]. For $N = 3$ it recovers Morgan's result, but for $N > 3$ it apparently has serious defects. The more involved but more powerful (§ 3–§ 8) starts from the original COST papers to which we return shortly. A major element is "geometric spectral analysis", i.e. the use of heavily geometric (configuration space) ideas to find the essential spectrum $\sigma_{\text{ess}}(H(f))$ of certain transforms $H(f)$ of H. Such ideas go back to Zhislin [32] and were developed by Jörgens and Weidmann [17], but their simplicity and power were realised only recently due to a paper of Enss [12]. The operators $H(f)$ will not be self-adjoint, so §3–§4 will be devoted to extend Enss'analysis to this case.

Simultaneously and independently of our work Alrichs and M. and T. Hoffmann-Ostenhof [3, 4] studied the atomic case (with fixed nucleus) and obtained similar results. One advantage of their method is that constants like C_α in (1.5)) are explicitely given numbers, while our constants are only implicitely determined depending, e.g., on norms of resolvents of non-normal operators which are difficult to control. Other methods giving explicit constants appear in Davies [10] (who only estimates $\|\psi\|_\infty$, not $\|\psi\exp(\alpha|x|)\|_\infty$ and requires $V_{ij}\geqq 0$) and Lavine [20] (who considered the case $N=2$).

Let us briefly describe the Combes-Thomas proof [9] of (1.3) since its extension will concern us here. (1.3) states that $\psi\exp(\alpha|x|)\in L^2(X)$ if $\alpha^2<\Sigma-E$, which is equivalent to $\psi\exp(a,x)\in L^2(X)$ for all $a\in X$ with $(a,a)=a^2<\Sigma-E$. Let $U(a)$, $a\in X$, be the group of unitary transformations $\psi(x)\to\psi(x)\exp(-i(a,x))$. Then $\psi\exp(a,x)\in L^2(X)$ for all a with $a^2<\Sigma-E$ if and only if the function $a\to U(a)\psi$ has an analytic continuation from the real space X to the region $(\operatorname{Im} a)^2<\Sigma-E$ of $\bar{X}$ $=$complexification of X. This reduces the proof of (1.3) to showing that ψ is an analytic vector for the group $U(a)$. For real a we have

$$U(a)HU^{-1}(a)=(p+a)^2+V\equiv H(a).$$

If V is H_0-bounded (or H_0-form-bounded), $H(a)$ extends to an entire analytic family of type (A) (or of type (B)) in the sense of Kato [18], defined for all $a\in\bar{X}$.

An argument of Combes [1, 5] now implies that a discrete eigenvalue E of H (i.e. an isolated eigenvalue of finite multiplicity) remains a discrete eigenvalue for $H(a)$ if there exists an open, connected set $N\subset\bar{X}$ containing 0 and a, such that $\sigma_{\text{ess}}(H(b))\not\ni E$ for all $b\in N$. For suppose that E is a discrete eigenvalue of $H(b_0)$, $b_0\in N$. Then E may split into eigenvalues $E_i(z)$ of $H(b_0+zb_1)$ which depend analytically [18] on z for small $|z|$, where $b_1\in X$ is arbitrary. However, since $H(b_0)$ and $H(b_0+zb_1)$ are unitarily equivalent for real z, $E_i(z)=E$ for $\operatorname{Im} z=0$ and therefore for all z in a neighbourhood of 0. Since b_1 is arbitrary, we conclude that E remains a discrete eigenvalue of $H(b)$ for b in a neighbourhood of b_0 and, by a continuation argument, for all $b\in N$. Similarly, the corresponding eigenprojection $P(b)$ is analytic in $b\in N$.

Analyticity of ψ now follows from a Lemma of O'Connor [23]: Let $P(b)$ be an analytic family of projections for b in an open, connected region $N\ni 0$ of $\bar{X}$. Suppose that $P(a+b)=U(a)^{-1}P(b)U(a)$ for $a\in X$, $b\in N$, $b+a\in N$. If $P(0)$ is of finite rank and $\psi\in\operatorname{Ran} P(0)$, then the function $b\to U(b)\psi$ has an analytic continuation from $X\cap N$ to N.

This reduces the proof of (1.3) to showing that $E\notin\sigma_{\text{ess}}(H(a))$ for $(\operatorname{Im} a)^2<\Sigma-E$. Using "connected" resolvent equations for $(z-H(a))^{-1}$, Combes and Thomas prove that (in the notation of Appendix 1)

$$\sigma_{\text{ess}}(H(a))=\bigcup_D\{\Pi_D(p+a))^2+\Sigma_D|p\in X\}$$

where D runs over all partitions of $(1 \ldots N)$ into more than one cluster. In particular, $E \notin \sigma_{\text{ess}}(H(a))$ so long as

$$(\Pi_D(\operatorname{Im} a))^2 < \Sigma_D - E \tag{1.6}$$

for all nontrivial D. Choosing D independently to make the left-hand side of (1.6) maximal ($\Pi_D = 1$) and the righthand side minimal ($\Sigma_D = \Sigma$) we obtain the single sufficient condition $(\operatorname{Im} a)^2 < \Sigma - E$ leading directly to (1.4). Therefore, by fully exploiting the Combes-Thomas analysis, one can already improve the COST estimates (1.3–5). To formulate the results we now collect the conditions on the potentials to which we will refer in this paper:

(C 1) Each V_{ik} viewed as an operator on $L^2(R^\nu)$ is $(-\Delta)$-form compact.

(C 2) Each V_{ik} viewed as a function on R^ν has a Fourier transform $\hat{V}_{ik} \in L^p(R^\nu) + L^1(R^\nu)$ with $p < \nu(\nu-2)^{-1}$ if $\nu \geqq 2$ or $p \leqq \infty$ if $\nu = 1$.

(C 3) Each V_{ik} viewed as a function on R^ν obeys $V_{ik} \in L^p(R^\nu) + L^\infty(R^\nu)$ and $V_{ik}(y) \to 0$ as $|y| \to \infty$, where $p > \nu/2$ if $\nu \geqq 4$ or $p = 2$ if $\nu = 1, 2, 3$.

Most of the results in this paper will be proven for potentials satisfying (C 3). (C 1) follows from (C 2) or (C 3) and is sufficient for the Combes-Thomas analysis [9]. (C 2) is the condition used by Simon [26] to go from (1.3) to (1.5) by showing, essentially, that if an eigenfunction ψ of H satisfies $\psi \exp(a, x) \in L^2$ for some $a \in X$ then $\psi \exp(a, x) \in L^\infty$. This together with (1.6) immediately gives Theorem 1.1 below.

Definition. Let ψ be a complex function on X. A positive function f on X is called an L^p exponential bound for ψ if and only if $\psi \exp(\varkappa f) \in L^p(X)$ for all $\varkappa < 1$.

Theorem 1.1 *(Improved COST). Let H be an N body Hamiltonian obeying* (C 1) *and let $H\psi = E\psi$. If $a \in X$ satisfies the conditions* (1.6) *for all nontrivial D, then $f(x) = (a, x)$ is an L^2 exponential bound. If* (C 2) *holds, f is an L^∞ exponential bound.*

Example 1.1. Consider 3 particles 0, 1, 2 with $m_0 = \infty$ ($x^0 = 0$, $x^{1,2}$ independent coordinates). Let $\Sigma_0, \Sigma_1, \Sigma_2$ be the lowest energies of the subsystems (12), (02), (01), respectively. According to (1.3), $f(x) = (a, x) = a_1 x^1 + a_2 x^2$ is an exponential bound if

$$a_1^2(2m_1)^{-1} + a_2^2(2m_2)^{-1} \leqq \min_i (\Sigma_i - E), \tag{1.3'}$$

which should be compared with the following 4 inequalities:

$$a_i^2(2m_i)^{-1} \leqq \Sigma_i - E \quad (i = 1, 2) \tag{1.6'a}$$

$$(a_1 + a_2)^2(2m_1 + 2m_2)^{-1} \leqq \Sigma_0 - E \tag{1.6'b}$$

$$a_1^2(2m_1)^{-1} + a_2^2(2m_2)^{-1} \leqq -E \tag{1.6'c}$$

obtained from (1.6) for the 4 decompositions $D = (02)(1), (01)(2), (0)(12), (0)(1)(2)$ in this order. (1.6′) can be much weaker than (1.3′), e.g. if $\Sigma_0 = \Sigma_2 = 0$ and if $(E/\Sigma_1) - 1$ is small, then (1.3′) forces both a_1 and a_2 to be small while (1.6′) only forces a_1 to be small.

Notice that, if $\Sigma_0=0$, (1.6′c) implies (1.6′b) since

$$a_1^2(2m_1)^{-1}+a_2^2(2m_2)^{-1}-(a_1+a_2)^2(2m_1+2m_2)^{-1}$$
$$=m_1m_2(2m_1+2m_2)^{-1}(a_1m_1^{-1}-a_2m_2^{-1})^2\geqq 0\,.$$

This is actually a special case of

Lemma 1.2. *Let $D\lhd D'$ and suppose that $\Sigma_D=\Sigma_{D'}$ (in general $\Sigma_D\leqq\Sigma_{D'}$). Then* (1.6) *for D' implies* (1.6) *for D.*

Proof. Since $D\lhd D'$ implies the operator inequality $\Pi_D\leqq\Pi_{D'}$ (A 1.5), it follows that $(\Pi_D a)^2\leqq(\Pi_{D'}a)^2$. □

The L^∞ exponential bound one gets from (1.6) by optimizing over a for fixed x is the Minkowski functional

$$f(x)=\sup\{(a,x)|a \text{ obeying } (1.6)\}$$

of the polar of the convex set of a's defined by (1.6). This suggests that one should search for exponential bounds f which are positive and homogeneous of degree 1. The Combes-Thomas argument has an immediate extension to this case: instead of $H(a)$ consider

$$e^{-if}He^{+if}=(p+\nabla f)^2+V\equiv H(f)\,. \tag{1.7}$$

If $H\psi=E\psi$ and $E\notin\sigma_{\text{ess}}(H(i\lambda f))$ for $0\leqq\lambda<1$ then f is an L^2 exponential bound for ψ. The problem of expressing $\sigma_{\text{ess}}(H(f))$ in terms of the function f and of the thresholds and the masses will be solved in § 3, 4. In § 5 we state the resulting sufficient conditions for f to be an L^2 exponential bound. The corresponding L^∞ exponential bounds are derived in § 6. Inspection of the proof in [26] shows that it extends in a straightforward way to *convex* exponents $f(x)$. The functions f of interest, however, will not be convex, but they are *Lipschitz*. This will be used in § 6 to prove:

Theorem 1.3. *Let H be an N body Hamiltonian obeying* (C 3) *and let $H\psi=E\psi$. Suppose that f is an L^2 exponential bound for ψ. If*

$$|f(x)-f(y)|\leqq a|x-y|$$

for all, $x,y\in X$, then f is an L^∞ exponential bound for ψ.

The resulting L^∞ bounds will be dubbed "ultimate COST estimates" since they are obtained by extending the COST ideas to their natural but ultimate extremum. In § 7–8 we construct explicit exponential bounds f for atoms with infinite nuclear mass and for general 3-particle systems. Due to the kinematical complexity, the problem remains open to find the optimal bound f consistent with the conditions of § 5 for a general N-particle system with given masses and thresholds.

We close this introduction with a comment about the use of the word "best possible" with regard to exponential bounds. We have learned to use the word sparingly. The actual behaviour of bound state wave functions at infinity seems to depend in an intricate way on relations among the thresholds and the masses, so that a result which is "best possible" in a particular example (e.g. an "atom" with noninteracting electrons) may not be optimal in other cases.

§ 2. Comparison Theorem Methods

In this section we present a method which in particular yields Morgan's result for the Helium atom. The basic result we need is the following comparison theorem:

Theorem 2.1. *Let* $\varphi \geqq 0$ *and* ψ *be continuous and* $A \geqq B \geqq 0$ *on* $\overline{R^n \backslash S}$ *for some closed set* S. *Suppose that on* $R^n \backslash S$, *in the distributional sense,*

$$\Delta|\psi| \geqq A|\psi|\,; \qquad \Delta\varphi \leqq B\varphi \tag{2.1}$$

and that $|\psi| \leqq \varphi$ *on* ∂S *and* $\psi, \varphi \to 0$ *as* $x \to \infty$. *Then* $|\psi| \leqq \varphi$ *on all of* $R^n \backslash S$.

Remark. This theorem is used in [27] where references to earlier work can be found. A variant of it also serves as the basic tool in the recent independent work of Alrichs, M. and T. Hoffmann-Ostenhof [4]. Its proof is so short that we repeat it here:

Proof. Let $\eta = |\psi| - \varphi$ and $K = \{x \mid \eta(x) > 0\}$. Then on the open set K, $\Delta\eta \geqq A|\psi| - B\varphi = (A-B)\varphi + A(|\psi| - \varphi) \geqq 0$. So η is subharmonic and therefore takes its maximum value on $\partial K \cup \{\infty\}$ where it vanishes by hypothesis. Thus $\eta \leqq 0$ on $\bar{K}$. Since $\eta > 0$ on K, K is empty. □

To combine this result with COST, we use geometric ideas which already dominate some of our recent work on N-body systems [11, 28]. We isolate tubes in X around the sets $x^i = x^j$. Then we will pick a φ which dominates the COST estimate for ψ on these tubes, so that there we have $|\psi| \leqq \varphi$. By making the tubes sufficiently fat we will be sure that outside their union S, $V \geqq -\delta \geqq E$ and by Kato's inequality [19, 24]

$$\Delta|\psi| \geqq (V-E)|\psi| \geqq (-E-\delta)|\psi| \tag{2.2}$$

on $R^n \backslash S$. Then, if φ obeys $\Delta\varphi \leqq (-\varphi - E)\varphi$ we will have $|\psi| \leqq \varphi$ on all of X.

Theorem 2.2. *Let* H *be an* N-*body Hamiltonian obeying* (C 2) *and with* $V_{ij}(x) \to 0$ *for* $x \to \infty$ *in* R^ν. *For* $i \neq j$ *let* D_{ij} *be the partition of* $(1 \ldots N)$ *into the* $N-1$ *clusters* (ij) *and* (k), $k \neq i, j$.

Let

$$z_{ij} = |(1 - \Pi_{D_{ij}})x| = \sqrt{2}(m_i^{-1} + m_j^{-1})^{-1/2}|x_i - x_j|$$

$$y_{ij} = |\Pi_{D_{ij}} x| = (x^2 - z_{ij}^2)^{1/2}\,.$$

Let $H\psi = E\psi$, $E < \Sigma$, *and for each* $\varepsilon > 0$ *let*

$$\varphi_{ij}^{(\varepsilon)}(x) = \exp\{-(1-\varepsilon)[y_{ij}(\Sigma - E)^{1/2} + z_{ij}(-\Sigma)^{1/2}]\}\,.$$

Then

$$|\psi(x)| \leqq C(\varepsilon) \sum_{i<j} \varphi_{ij}^{(\varepsilon)}(x) \equiv \varphi^{(\varepsilon)}(x)\,. \tag{2.3}$$

Proof. Let $S_{ij} = \{x \mid z_{ij} \leqq y_{ij}^{1/2}\}$ and $S_0 = \{x \mid x^2 \leqq R^2\}$ where the constant R will be adjusted below. Let $S = S_o \cup \bigcup S_{ij}$. On S_{ij}, $|\psi(x)| \leqq C(\varepsilon)\varphi_{ij}^{(\varepsilon)}$ by (1.5) and clearly $|\psi| \leqq \varphi^{(\varepsilon)}$ on S_0 for suitable $C(\varepsilon)$. Thus (2.3) holds on S and, in particular, on ∂S. To obtain (2.1) for suitable A and B with $A \geqq B \geqq 0$ we first claim that on $R^n \backslash S$,

$z_{ij} \geqq \alpha(R) \to \infty$ as $R \to \infty$. This follows from noting that on $R^n \backslash S$, $R^2 \leqq x^2 = z_{ij}^2 + y_{ij}^2 \leqq z_{ij}^2 + z_{ij}^4$ and therefore $z_{ij}^2 \geqq (R^2 + 1/4)^{1/2} - 1/2$. Given $\delta > 0$ we can therefore pick R so that

$$V(x) \geqq -\delta \tag{2.4}$$

on $R^n \backslash S$. It follows from (2.2) that $\Delta|\psi| \geqq (-E-\delta)|\psi|$ on $R^n \backslash S$.

Next, using that for a function $f(r)$ of the radius $r=|x|$ in R^n, $(\Delta f)(r) = d^2f/dr^2 + (n-1)r^{-1}df/dr$, we see that $\Delta(e^{-ar}) = a^2e^{-ar} - a(n-1)r^{-1}e^{-ar} \leqq a^2e^{-ar}$ for $n>1$, and also for $n=1$ since $\Delta(e^{-ar}) = a^2e^{-ar} - a\delta(r)e^{-ar} \leqq a^2e^{-ar}$. On X, $\Delta = \Delta_{y_{ij}} + \Delta_{z_{ij}}$ and we see that

$$\Delta\varphi^{(\varepsilon)} \leqq -E(1-\varepsilon)^2\varphi^{(\varepsilon)}.$$

Since $E<0$, we can choose $\delta>0$ such that $-E-\delta > -E(1-\varepsilon)^2$, so that (2.1) holds with $A=-E-\delta$ and $B=-E(1-\varepsilon^2)$. Noting that $\varphi^{(\varepsilon)}(x) \to 0$ and by (1.5) also $\psi(x) \to 0$ as $x \to \infty$, we see that (2.3) follows from Theorem 2.1. □

Notice that if some $V_{ij} \geqq 0$, then (2.2) holds even if the corresponding z_{ij} are not large. Thus we have:

Corollary 2.3. *Under the hypothesis of Theorem 2.2, the estimate* (2.3) *remains valid if we defer from the sum all terms coming from pairs* (ij) *with* $V_{ij} \geqq 0$.

Example 2.1. (2 electron atom, finite nuclear mass). Take 3 particles 0, 1, 2 with $V_{01} = V_{02}$ and $V_{12} \geqq 0$. Then by (2.3) and Corollary 2.3:

$$|\psi(x)| \leqq C(\varepsilon)[e^{-(1-\varepsilon)f_1} + e^{-(1-\varepsilon)f_2}] \quad \text{with}$$

$$f_1(x) = (2(\Sigma - E)M)^{1/2}|x^1 - (m_0+m_2)^{-1}(m_0x^0 + m_1x^1)| + (-2\Sigma\mu)^{1/2}|x^2 - x^0|$$

where $\mu^{-1} = m_0^{-1} + m_2^{-1}$, $M^{-1} = m_1^{-1} + (m_0+m_2)^{-1}$ and where f_2 is obtained by interchanging 1 and 2. This is Morgans bound [22].

Example 2.2. (N electron atom, infinite nuclear mass). Take $N+1$ particles $0, 1, \ldots, N$ with $m_0 = \infty$, $m_1 = \ldots m_N = 1/2$, and suppose that $V_{0i}(x)$ and $0 \leqq V_{ij}(x)$ are independent of $i, j = 1 \ldots N$. Let $E \equiv E_N < E_{N-1} \leqq E_{N-2} \ldots \leqq E_0 = 0$ where E_n = lowest energy of the subsystem $(0, 1, \ldots, n)$ for $n = 0, 1, \ldots N-1$. For comparison with Example 7.2 (§ 7) let us assume (7.6). Then $E_{N-1} - E_N \leqq E_{N-2} - E_{N-1} \leqq -E_{N-1}$ and Corollary 2.3 gives the L^∞ exponential bound $f(x)$, where f is symmetric in $x^1 \ldots x^N$ and reduces to

$$f = r_1(-E_{N-1})^{1/2} + (r_2^2 + \ldots + r_N^2)^{1/2}(E_{N-1} - E_N)^{1/2}$$

on the sector $r_1 \leqq r_2 \ldots \leqq r_N (r_i = |x^i|)$. For $N=2$ this agrees with the bound given in Example 7.2, but for $N>2$ it is seen to be smaller:

Lemma 2.4. *If* $0 \leqq a_1 \leqq \ldots \leqq a_n$ *and* $b_1 \geqq b_2 \geqq \ldots \geqq b_n \geqq 0$, $n \geqq 2$, *then*

$$\sum_{i=1}^{n} a_i b_i \geqq a_1 \left(\sum_{i=1}^{n-1} b_i^2\right)^{1/2} + b_n \left(\sum_{i=2}^{n} a_i^2\right)^{1/2} \equiv g(a,b).$$

Proof. Fix the b's and a_1. Then the inequality holds for $a_2 = \dots = a_N = a_1$, since

$$g(a,b) = a_1 \left[(n-1)^{1/2} b_n + \left(\sum_{i=1}^{n-1} b_i^2 \right)^{1/2} \right] \leqq a_1 \sum_{i=1}^{n} b_i .$$

Therefore it suffices to prove $\partial g / \partial a_k \geqq b_k$ for $k = 2 \dots n$:

$$\partial g / \partial a_k = a_k b_n \left(\sum_{i=2}^{n} a_i^2 \right)^{-1/2} \leqq b_n \leqq b_k . \quad \square$$

In cases where the 2 cluster thresholds are not all at Σ, one can hope to improve Theorem 2.2 by using Theorem 1.1. Possibly one could obtain the full Mercuriev-type result (§ 8) for $N=3$, but because of the global nature of the conditions (1.6) the kinematics is fierce. We settle for:

Example 2.3 (same situation as in Example 1.1). Suppose that $V_{12} \geqq 0$ and that $m_1 = m_2 = 1/2$ for kinematic simplicity. By (1.6′) and optimizing over a we have the 2 exponential bounds

$$f_i(x) = |x^i| (\Sigma_i - E)^{1/2} \qquad (i = 1, 2) .$$

Using the method of proving Theorem 2.2 and Corollary 2.3 we find the L^∞ exponential bound

$$f(x) = \min_{i=1,2} \left[|x^i| (\Sigma_i - E)^{1/2} + |x^j| (-\Sigma_j)^{1/2} \right]$$

where $j = 2, 1$ *for* $i = 1, 2$.

We close by noting one way of further improving Theorem 2.2 by a device that will also prove useful in §7:

Definition. For $x, y, \alpha, \beta \geqq 0$ we define the Mercuriev function M by

$$M(x, y; \alpha, \beta) = \begin{cases} x\alpha + y\beta & \text{if } \; y\alpha \geqq x\beta \\ (x^2+y^2)^{1/2} (\alpha^2+\beta^2)^{1/2} & \text{if } \; y\alpha \leqq x\beta \end{cases}$$

Noting that $G(x,y) \equiv (x^2+y^2)^{1/2} (\alpha^2+\beta^2) - x\alpha - y\beta \geqq 0$ for all x, y we see that $\nabla G(x,y) = 0$ for $G(x,y) = 0$ (i.e. for $y\alpha = x\beta$). Thus M is a C^1 function of x, y. As a result (in the notation of Theorem 2.2), the functions

$$M(z_{ij}, y_{ij}; (-\Sigma)^{1/2}, (\Sigma - E)^{1/2}) \equiv M_{ij}(x)$$

obey, in the distributional sense,

$$\Delta e^{-(1-\varepsilon) M_{ij}} \leqq -E (1-\varepsilon)^2 e^{-(1-\varepsilon) M_{ij}} ,$$

since the C^1-nature of M_{ij} prevents δ-function singularities on the "matching surfaces". Thus we obtain:

Theorem 2.5. *Under the hypothesis of Theorem* 2.2, (2.3) *remains valid if*

$$\varphi_{ij}^{(\varepsilon)} \quad \textit{is replaced by} \quad \exp(-(1-\varepsilon) M_{ij}) .$$

With this device we have improved individual terms of the sum (2.3) in certain regions. Whether this improves the sum or not depends on relations among the thresholds and the masses. In §7 we will see that for atoms, it does not.

The above examples still show two defects in the method of this section: (i) it seems only effective under removing the first particle and the last and therefore not ideal for $N>3$ (This difficulty was recently overcome by Alrichs, M. and T. Hoffmann-Ostenhof [4]); (ii) because of the global nature of the improved COST conditions (1.6), it is not easy to check with complicated kinematics. In distinction, the second method which we now describe is efficient for arbitrary N and yields local conditions for f.

§ 3. Weyl's Criterion for the Essential Spectrum

In this section we prepare the tools for the determination of $\sigma_{\text{ess}}(H(f))$. Let A be a closed operator on a Hilbert space $\mathscr{H}$ with resolvent set $\varrho(A)$ and spectrum $\sigma(A)$.

Definition [25]. $\sigma_{\text{disc}}(A)=$ set of all isolated eigenvalues of A with finite algebraic multiplicities.

$$\sigma_{\text{ess}}(A)=\sigma(A)\backslash\sigma_{\text{disc}}(A).$$

Definition. $N_{\text{ess}}(A)=\{\lambda\in C \mid \text{There exists a sequence } u_n\in D(A) \text{ such that } \|u_n\|=1,$ $u_n\to 0 \text{ (weakly) and } \|(\lambda-A)u_n\|\to 0\}.$

We remark that $N_{\text{ess}}(A)$ is closed.

Theorem 3.1. *(Weyl's criterion for $\sigma_{\text{ess}}(A)$). Let A be a closed operator on $\mathscr{H}$ with nonempty resolvent set. Then*

(i) $N_{\text{ess}}(A)\subset\sigma_{\text{ess}}(A)$

(ii) *Boundary of* $\sigma_{\text{ess}}(A)\subset N_{\text{ess}}(A)$

(iii) $N_{\text{ess}}(A)=\sigma_{\text{ess}}(A)$ *if and only if each connected component of the complement of* $N_{\text{ess}}(A)$ *contains a point of* $\varrho(A)$.

Remarks. 1. (iii) is an immediate corollary of (i) and (ii)

2. Examples where $N_{\text{ess}}(A)=\sigma_{\text{ess}}(A)$ are the case $A=A^*$, or cases where the complement of $N_{\text{ess}}(A)$ is connected.

3. A proof of Theorem 3.1 is implicit in [18], Theorems IV 5.11, IV 5.28 and problem IV 5.37. (Note that Kato's definition of the essential spectrum $\Sigma_e(A)$ differs from ours.) A proof of the Banach space version is also given in [26]. Ideas like (ii), but for the full spectrum $\sigma(A)$, are a standard tool in operator theory, see e.g. [7].

In quantum mechanics, Weyl's criterium was first used by Zhislin [32] to determine $\sigma_{\text{ess}}(H)$. Recently, Enss [12] has given a very elegant variant of this method which we describe below, extending it to the case of non-selfadjoint operators which concerns us here:

Let X be a real, finite dimensional, normed vector space, equipped with Lebesgue measure. In the following, A is a closed operator on $L^2(X)$ having $C_0^\infty(X)$ as a core.

Definition. $N_\infty(A)=\{\lambda\in C|$There exists a sequence $u_n\in C_0^\infty(X)$ such that $\|u_n\|=1$, $\operatorname{supp}u_n\cap K$ empty for each compact $K\subset X$ and n sufficiently large, and $\|(\lambda-A)u_n\|\to 0$ as $n\to\infty\}$. We will call a sequence u_n of this type a *Weyl sequence for* A *and* λ.

Clearly $N_\infty(A)\subset N_{\text{ess}}(A)$. Following Enss [12] we obtain sufficient conditions for the converse:

Theorem 3.2. *Let A be a closed operator on $L^2(X)$ with nonempty resolvent set, having $C_0^\infty(X)$ as a core. Let $X_0\in C_0^\infty(X)$, $X_0(X)=1$ for x in a neighbourhood of 0, and let X_0^d be the operator of multiplication by $X_0(x/d)$ for $0<d<\infty$. Suppose that for each d, $X_0^d(z-A)^{-1}$ is compact for some (and hence all) $z\in\varrho(A)$, and that for all $u\in C_0^\infty(X)$*

$$\|[A,X_0^d]u\|\leqq\varepsilon(d)(\|Au\|+\|u\|) \tag{3.1}$$

with $\varepsilon(d)\to 0$ as $d\to\infty$. Then $N_\infty(A)=N_{\text{ess}}(A)$.

Proof. Let $\lambda\in N_{\text{ess}}(A)$. By definition, there exists a sequence $u_n\in D(A)$ with $\|u_n\|=1$, $u_n\to 0$ (weakly) and $\|(\lambda-A)u_n\|\to 0$. Since $C_0^\infty(X)$ is a core of A, we may assume that $u_n\in C_0^\infty(X)$. Then, for $z\in\varrho(A)$,

$$\|X_0^d u_n\|=\|X_0^d(z-A)^{-1}(z-A)u_n\|\to 0$$

as $n\to\infty$, since by hypothesis $X_0^d(z-A)^{-1}$ is compact and $(z-A)u_n\to 0$ (weakly). By (3.1)

$$\|(\lambda-A)(1-X_0^d)u_n\|\leqq\|(\lambda-A)u_n\|+\varepsilon(d)(\|Au_n\|+1).$$

Taking $d=1,2,\ldots$ we can therefore pick a subsequence $n(d)$ of $\{n\}$ such that $\|(1-X_0^d)u_{n(d)}\|\to 1$ and $\|(\lambda-A)(1-X_0^d)u_{n(d)}\|\to 0$ as $d\to\infty$. For any compact $K\subset X$, $\operatorname{supp}(1-X_0^d)\cap K$ is empty for d sufficiently large, hence $\lambda\in N_\infty(A)$. □

For the analysis of Schrödinger Hamiltonians in configuration space we need more detailed control over $\operatorname{supp}u_n$:

Definition. A *partition of unity on* X is a finite set $X_0\ldots X_s$ of C^∞ functions on X with bounded derivatives obeying:

$$0\leqq X_i\leqq 1;\ \sum_{i=0}^{s}X_i=1$$

$X_0\in C_0^\infty(X)$; $X_0=1$ on some neighbourhood of 0. For $0<d<\infty$, X_i^d denotes the function $X_i(x/d)$ and also the corresponding multiplier on $L^2(X)$.

Definition. Let $X_0\ldots X_s$ be a partition of unity on X. For $i=1\ldots s$ we define $N_\infty^i(A)=\{\lambda\in C|$There exists a Weyl sequence u_n for A and λ with $\operatorname{supp}u_n\subset\operatorname{supp}X_i^n\}$.

Clearly $N_\infty^i(A)\subset N_\infty(A)$ for $i=1\ldots s$. Again we can state a converse which, combined with Theorems 3.1 and 3.2, gives a possible characterisation of $\sigma_{\text{ess}}(A)$:

Theorem 3.3. (i) *Let A be a closed operator on $L^2(X)$ having $C_0^\infty(X)$ as a core. Let $X_0\ldots X_s$ be a partition of unity and suppose that for all $u\in C_0^\infty(X)$ and $i=1\ldots s$*

$$\|[A,X_i^d]u\|\leqq\varepsilon(d)(\|Au\|+\|u\|) \tag{3.2}$$

with $\varepsilon(d)\to 0$ *as* $d\to\infty$. *Then*

$$N_\infty(A)=\bigcup_{i=1}^{s} N^i_\infty(A).$$

(ii) *If, in addition,* A *and* X_0 *satisfy the hypothesis of Theorem 3.2, then*

$$N_{\mathrm{ess}}(A)=\bigcup_{i=1}^{s} N^i_\infty(A).$$

(iii) *If, moreover, the complement of* $N_{\mathrm{ess}}(A)$ *is connected, then*

$$\sigma_{\mathrm{ess}}(A)=\bigcup_{i=1}^{s} N^i_\infty(A).$$

Proof. Let $\lambda\in N_\infty(A)$ and let u_n be a corresponding Weyl sequence. Without loss of generality we may assume that $X^n_0 u_n=0$, so that

$$u_n=\sum_{i=1}^{s} X^n_i u_n.$$

Therefore

$$\|X^m_i u_m\|\leqq s^{-1}>0 \tag{3.3}$$

for some index $i\in(1\ldots s)$ and for an infinite subsequence $\{m\}$ of $\{n\}$. By (3.2)

$$\|(\lambda-A)X^m_i u_m\|\leqq\|(\lambda-A)u_m\|+\varepsilon(m)(\|Au_m\|+1)\to 0$$

as $m\to\infty$. This together with (3.3) shows that $\lambda\in N^i(A)$. The remaining statements follow directly from Theorems 3.1 and 3.2. □

As an illustration of the simplicity and power of Theorem 3.3 we describe its use for the determination of $\sigma_{\mathrm{ess}}(H)$ [12] where H is the N-particle Hamiltonian with potentials obeying (C 3):

The three ingredients of Theorem 3.3 are:
(i) *Compactness.* For any $X_0\in C^\infty_0(X)$, $X_0(i+H_0)^{-1}$ is compact and, since $V(i+H)^{-1}$ is bounded, $X_0(i+H)^{-1}=X_0(i+H_0)^{-1}-X_0(i+H_0)^{-1}V(i+H)^{-1}$ is also compact.
(ii) *Commutator Estimates.* For local potentials the estimates (3.1) (3.2) involve only H_0, and $\varepsilon(d)$ is easily seen to be of order d^{-1}. (Note that by (C 3), H_0 is H-bounded).
(iii) *Partition of Unity.* Let $D=(C_1,C_2)$ run over all 2-cluster decompositions. Construct a partition of unity $X_0\cup\{X_D\}$ on X such that $\operatorname{dist}(C_1,C_2)>1$ for $x\in\operatorname{supp}X_D$. Then $\operatorname{dist}(C_1,C_2)>d$ for $x\in\operatorname{supp}X^d_D$ and it follows from (C 3) that $\|(H-H_D)u_n\|\to 0$ for any sequence $u_n\in C^\infty_0(X)$ with $\|u_n\|=1$ and $\operatorname{supp}u_n\subset\operatorname{supp}X^n_D$. Therefore $N^D_\infty(H)\subset N^D_\infty(H_D)$ and by Theorem 3.3

$$\sigma_{\mathrm{ess}}(H)=\bigcup_D N^D_\infty(H)\subset\bigcup_D N^D_\infty(H_D)\subset\bigcup_D \sigma(H_D). \tag{3.4}$$

Conversely, $\sigma(H_D)\subset\sigma_{\mathrm{ess}}(H)$ by a simple application of Weyl's criterion for the *full* spectrum: if $\lambda\in\sigma(H_D)$ there exists a sequence $u_n\in C^\infty_0(X)$ such that $\|u_n\|=1$ and $\|(\lambda-H_D)u_n\|\to 0$. For any $a\in X$ with $a=\Pi_D a$, $U(a):\psi(x)\to\psi(x-a)$ represents a relative translation of the clusters C_1,C_2 and commutes with H_D. Hence $\|(\lambda-H_D)v_n\|\to 0$ for $v_n=U(a_n)u_n$ and for any sequence $a_n=\Pi_D a_n$. Picking a_n such that $\operatorname{dist}(C_1, C_2) > n$ for $x \in \operatorname{supp} v_n$ we have $\|(H - H_D)v_n\| \to 0$. It follows that $\|(\lambda - H)v_n\| \to 0$, hence $\lambda \in \sigma(H)$. Combined with (3.4) we obtain

$$\sigma_{\text{ess}}(H) = \bigcup_{D=(C_1, C_2)} \sigma(H_D). \tag{3.5}$$

§ 4. Geometric Spectral Analysis of *H* (*f*)

In this section we apply Theorem 3.3 to express $\sigma_{\text{ess}}(H(f))$ in terms of the function f and of the thresholds and the masses. The idea is, essentially, to analyze the local operator $H(f)$ along fixed directions in configuration space. To formulate the result (Theorem 4.1) we introduce the following notions:

Definitions. (i) Let f be a complex C^∞ function on X satisfying $f(\lambda x) = \lambda f(x)$ for $|x| \geqq 1$ and $\lambda \geqq 1$. If H is the N-particle Hamiltonian we define:

$$H(f) = e^{-if} H e^{if} = (p + \nabla f)^2 + V.$$

(ii) For any $x \in X$ we define the cluster decomposition $D(x)$ as follows: two particles i and k belong to the same cluster if and only if $x^i = x^k$. If $x \neq 0$, $D(x)$ is nontrivial and depends only on the direction of x. Similarly, $\nabla f(x)$ is homogeneous of degree zero for $|x| \geqq 1$. To express this we introduce

$$\Omega = \{e \in X \mid |e| = 1\}$$

and the functions

$$D(e);\ a(e) \equiv (\nabla f)(e)$$

on the unit sphere Ω.
(iii) For any $a \in \bar{X}$ we set

$$H(a) = e^{-i(a,x)} H e^{i(a,x)} = (p + a)^2 + V,$$

and for any cluster decomposition D:

$$H_D(a) = e^{-i(a,x)} H_D e^{i(a,x)}$$
$$= H(a) - (\text{all intercluster potentials}).$$

Remarks. (i) If the potentials obey the condition (C 3) of §1, each of the operators $A = H(f)$, $H(a)$, $H_D(a)$ is defined on $C_0^\infty(X)$, where the norms $\|Au\| + \|u\|$ are all equivalent to $\|H_0 u\| + \|u\|$. Therefore each A has a closure (again denoted by A) with domain $D(A) = D(H_0)$ and satisfies the hypothesis of Theorem 3.3 (i) and (ii).
(ii) In the sense of (A 1.4) $H_D(a)$ can be expressed as

$$H_D(a) = H_D^0(a_D) + \sum_{C \in D} H_C(a_C),$$

where $a_D = \Pi_D a$, $a_C = \Pi_C a$. $H_C(a_C)$ is the exact analogue of $H(a)$ for the subsystem C. $H_D^0(a_D) = (\Pi_D(p + a))^2$ is a multiplier in p-space whose spectrum for nontrivial D is the parabolic region shown in Figure 1 (except for the case of particles in one dimension ($\nu = 1$), where for 2-cluster decompositions this region reduces to the

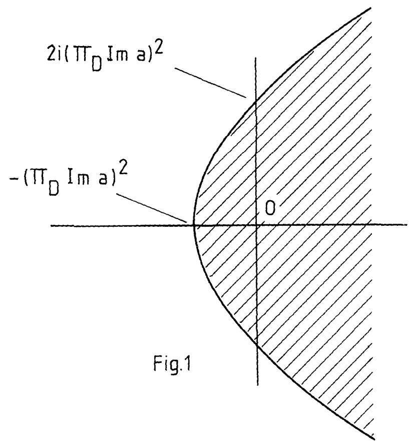


Fig.1

boundary parabola. For simplicity we disregard this exception in the following). By Ichinoses lemma [25]:

$$\sigma(H_D(a))=\sigma(H_D^0(a_D))+\sum_{C\in D}\sigma(H_C(a_C)). \tag{4.1}$$

Theorem 4.1. *If H is an N-particle Hamiltonian with potentials obeying* (C 3) *and if $v\geqq 2$, then*

$$\sigma_{\text{ess}}(H(f))=\bigcup_{e\in\Omega}\sigma[H_{D(e)}(a(e))].$$

Discussion. Setting $f=0$ we recover

$$\sigma_{\text{ess}}(H)=\bigcup_D\sigma(H_D)$$

where D runs over all nontrivial partitions. Choosing $f(x)=(a,x)$ for any $a\in\bar{X}$ we obtain

$$\sigma_{\text{ess}}(H(a))=\bigcup_D\sigma(H_D(a)).$$

Using (4.1) it follows from this by induction that for nontrivial D

$$\sigma(H_D(a))=\bigcup_{D'\trianglerighteq D}[\Sigma_{D'}+\sigma(H_{D'}^0(a_{D'}))]. \tag{4.2}$$

We conclude that Theorem 4.1, together with (4.2) and Fig. 1, completely describes $\sigma_{\text{ess}}(H(f))$ in terms of f and of the thresholds and the masses. In particular

$$\inf\operatorname{Re}\sigma_{\text{ess}}(H(f))=\inf_{e\in\Omega;\,D\trianglerighteq D(e)}[\Sigma_D-(\Pi_D\operatorname{Im}a(e))^2]. \tag{4.3}$$

This is the basic result from which the exponential bounds will be derived in § 5–8. We mention without proof that (4.3) remains true in the exceptional case $v=1$.

The proof of Theorem 4.1 is given in the remaining part of this section. In order to apply Theorem 3.3 we introduce the family of cones

$$K_\varepsilon(e)=\{x\in X\,|\,(e,x)>(1-\varepsilon)|x|\}$$

for $e\in\Omega$, $\varepsilon>0$, and for each $e\in\Omega$ the complex set

$$N_\infty(e)=\{\lambda\in C\,|\,\text{for any } \varepsilon>0 \text{ there exists a Weyl sequence } u_n \text{ for } H(a(e)) \text{ and } \lambda \text{ with } \operatorname{supp} u_n\subset K_\varepsilon(e)\}.$$

Since $H(f)$ resembles $H(a(e))$ on a narrow cone $K_\varepsilon(e)$ we expect as a limiting case of Theorem 3.3 (i):

Lemma 4.2. *Under the hypothesis of Theorem* 4.1,

$$N_\infty(H(f))=\bigcup_{e\in\Omega} N_\infty(e).$$

Proof. Let $u\in C_0^\infty(X)$ with $\operatorname{supp} u\subset K_\varepsilon(e)\cap\{|x|>R\}$ for $R>1$. Then

$$\begin{aligned}\|(H(f)-H(a))u\| &\leqq \|(\Delta f)u\|+\|((\nabla f)^2-a^2)u\|+2\|((\nabla f-a),p)u\|\\ &\leqq \alpha[R^{-1}+\beta(\varepsilon)]\,(\|H_0u\|+\|u\|),\end{aligned} \tag{4.4}$$

where α and $\beta(\varepsilon)$ depend only on f and $\beta(\varepsilon)\to 0$ as $\varepsilon\to 0$. (For ∇f is uniformly continuous, Δf is homogeneous of degree -1 for $|x|\geqq 1$ and p is H_0-bounded). Using this we first prove:

(i) $N_\infty(e)\subset N_\infty(H)f))$: Let $\lambda\in N_\infty(e)$. Then there exists a Weyl sequence u_n for $H(a(e))$ and λ with $\operatorname{supp} u_n\subset K_{1/n}(e)\cap\{|x|>n\}$. Since $\|H_0u_n\|$ is bounded for any Weyl sequence it follows from (4.4) that $\|(\lambda-H(f)u_n\|\to 0$; hence $\lambda\in N_\infty(H(f))$.

(ii) $N_\infty(H(f))\subset \bigcup_{e\in\Omega} N_\infty(e)$: Let $\lambda\in N_\infty(H(f)$. Given $\varepsilon>0$, $R>0$ we can choose $e\in\Omega$ and $u\in C_0^\infty(X)$, $\|u\|=1$, such that $\operatorname{supp} u\subset K_\varepsilon(e)\cap\{|x|>R\}$ and $\|(\lambda-H(f))u\|<\varepsilon$ (To see this, take a partition of unity χ_i with $\operatorname{supp}\chi_i\subset K_\varepsilon(e_i)\cap\{|x|>1\}$ for $i=1\dots s$ and suitable $e_i\in\Omega$ and apply Theorem 3.3 (i)). Making such a choice for each $(\varepsilon,R)=(n^{-1},n)$, $n=1,2,\dots$ we obtain sequences $u_n\in C_0^\infty(X)$ and $e_n\in\Omega$ with $\|u_n\|=1$, $\operatorname{supp} u_n\subset K_{1/n}(e_n)\cap\{|x|>n\}$ and

$$\|(\lambda-H(f))u_n\|<1/n. \tag{4.5}$$

Since Ω is compact we may, by passing to a subsequence, assume that $e_n\to e$. Then $K_{1/n}(e_n)\subset K_\varepsilon(e)$ for any $\varepsilon>0$ if n is sufficiently large. By (4.4) and (4.5) we conclude that

$$\|(\lambda-H(a(e))u_n\|\to 0$$

as $n\to\infty$, which proves that $\lambda\in N_\infty(e)$. □

Lemma 4.3. *Under the hypothesis of Theorem* 4.1 *we have for each* $e\in\Omega$

$$N_\infty(e)=\sigma[H_{D(e)}(a(e))].$$

Proof. Since e is fixed, we write $D(e)=D$, $a(e)=a$. We first prove:

(i) $N_\infty(e) \subset \sigma(H_D(a))$: Choose $\varepsilon > 0$ sufficiently small so that $|x^i - x^k| > \delta|x| (\delta > 0)$ for $x \in K_\varepsilon(e)$ and i, k in different clusters of D. Let $\lambda \in N_\infty(e)$ and let u_n be a Weyl sequence for $H(a)$ and λ with $\operatorname{supp} u_n \subset K(e) \cap \{|x| > n\}$. Then $\| V_{ik} u_n\| \to 0$ as $n \to \infty$ if i, k are in different clusters of D, and it follows that $\|(\lambda - H_D(a))u_n\| \to 0$.

(ii) $\sigma(H_D(a)) \subset N_\infty(e)$: If Theorem 4.1 is true, it follows that there is a simple Weyl criterion for the *full* spectrum of $H(f): \lambda \in \sigma(H(f))$ if and only if $\|(\lambda - H(f))u_n\| \to 0$ for a sequence $u_n \in C_0^\infty(X)$, $\|u_n\| = 1$. Using this we proceed by induction, assuming that Theorem 4.1 is proved for all subsystems of less than N particles. In (4.1), Weyl's criterion then holds for $\sigma(H_C(a_C))$ by induction hypothesis and for $\sigma(H_D^0(a_D))$ since $H_D^0(a_D)$ is a multiplier in p-space. Therefore it holds for $\sigma(H_D(a))$ since we may pick Weyl sequences of product form with respect to the factorization (A 1.3). So let $\lambda \in \sigma(H_D(a))$ and $u_n \in C_0^\infty$, $\|u_n\| = 1$, and

$$\|(\lambda - H_D(a))u_n\| \to 0$$

as $n \to \infty$. By definition of $D(e)$, translations of the form $x \to x + be$ $(b \in R)$ leave the configurations inside the clusters of D invariant, so that the corresponding unitary translation operators $U(be): u(x) \to u(x - be)$ commute with $H_D(a)$. Therefore

$$\|(\lambda - H_D(a))U(b_n e)u_n\| \to 0$$

for any choice of the sequence $b_n \in R$. Given $\varepsilon > 0$ and u_n we can always pick $b_n \in R$ such that $\operatorname{supp} U(b_n e)u_n \subset K_\varepsilon(e) \cap \{|x| > n\}$. This proves that $\lambda \in N_\infty(e)$. □

Proof of Theorem 4.1. By induction hypothesis Theorem 4.1 holds for all subsystems of less than N particles. Therefore $\sigma[H_{D(e)}(a(e))]$ is given by (4.2). According to Lemmas 4.2 and 4.3,

$$N_\infty(H(f)) = \bigcup_{e \in \Omega} \sigma[H_{D(e)}(a(e))],$$

which shows that the complement of $N_\infty(H(f)$ is connected. It follows from Theorem 3.3 that

$$\sigma_{\text{ess}}(H(f)) = N_\infty(H(f)). \quad \square$$

§ 5. L^2 Exponential Bounds

Combining the Combes-Thomas argument with the result (4.3) we see that f is an L^2 exponential bound for an eigenfunction ψ of H with energy E if

$$(\Pi_D a(e))^2 \leqq \Sigma_D - E \tag{5.1}$$

for all $e \in \Omega$ and for all $D \rhd D(e)$. In the derivation of (4.3) f was assumed to be a C^∞ function on X. In trying to find the largest possible f satisfying the gradient condition (5.1) we must be prepared, however, to encounter limiting functions f which are only piecewise smooth functions of x (such as the Mercuriev function occurring in Theorem 2.5). To cover this case we prove:

Theorem 5.1. *Let $H\psi = E\psi$, where H is an N-particle Hamiltonian obeying* (C3). *Then f is an L^2 exponential bound for ψ iff f is positive, continuous and homogeneous* *of degree* 1 *on* X *and if it has an* L^∞ *distributional gradient* $\nabla f = a$ *satisfying the following condition for all* $x \neq 0$:

$$(\Pi_D a(y))^2 \leqq \Sigma_D - E \tag{5.2}$$

for all $D \rhd D(x)$ *and almost all* y *in a neighbourhood* N_x *of* x.

Proof. We begin by noting that if we fix D, then $D(x) \lhd D$ if and only if $\Pi_D x = x$. As a result, if $\Omega = \{x \mid |x| = 1\}$, we see that $\{x \in \Omega \mid D(x) \lhd D\}$ is compact for each D and therefore, by a compactness argument, we can find $\delta > 0$ such that $N_x^0 \equiv \{y \mid |y - x| < \delta\} \subset N_x$ for all $x \in \Omega$. Let N be a neighbourhood of the identity in $SO(n)$ (viewed as the group of orthogonal transformations on X), such that $Rx \in N_x^0$ for $R \in N$ and $x \in \Omega$. Let j be a non-negative C^∞-function on $SO(n)$ with support in N and $\int j(R)\, dR = 1$ (dR = Haar measure). Then

$$f_j(x) = \int f(Rx) j(R)\, dR \tag{5.3}$$

is C^∞ and homogeneous of degree 1 on $X \setminus \{0\}$ since j smoothes in all nonradial directions. For $a_j = \nabla f_j$ we see that

$$(\Pi_D a_j(x))^2 \leqq \Sigma_D - E$$

for all $D \rhd D(x)$, since $j(R) \neq 0$ implies that $Rx \in N_x^0 \subset N_x$ and since the set $\{a \mid (\Pi_D a)^2 \leqq \Sigma_D - E\}$ is convex. Thus f_j is an exponential bound for ψ by (5.1).

Given ε in $0 < \varepsilon < 1$ and $\eta > 0$ we can choose j (near a δ-function on $SO(n)$) so that

$$(1-\varepsilon) f(x) \leqq (1-\varepsilon) f_j(x) + \varepsilon \eta |x| \tag{5.4}$$

for all x. By (5.1), $\eta|x|$ is an L^2 exponential bound if we choose $\eta^2 \leqq \Sigma - E$ (O'Connor's bound). Since the L^2 exponential bounds for ψ form a convex set, we conclude that $(1-\varepsilon) f$ is an exponential bound for any $\varepsilon > 0$, hence f is an exponential bound. □

§ 6. L^∞ Exponential Bounds

In this section we prove Theorem 1.3 which implies that the L^2 exponential bounds f derived in § 5 are also L^∞ exponential bounds. Having shown that $e^f \psi \in L^2$ is an eigenfunction with eigenvalue E of

$$e^f H e^{-f} = H(if) \tag{6.1}$$

it suffices to prove that $\exp(-tH(if))$ is bounded from L^2 to L^∞ for some $t > 0$, since then

$$e^{-tE} e^f \psi = e^{-tH(if)} e^f \psi \in L^\infty . \tag{6.2}$$

We will prove this property of $\exp(-tH(if))$ for all $t > 0$ (By keeping track of the rate of divergence of the operator norm as $t \to 0$ one could show more generally that for suitable n, $e^f \psi \in D(H(if)^n)$ implies $e^f \psi \in L^\infty$. For the case $f = 0$ this is done in § 25 of [29]).

Most of the ideas in the proof go back to Herbst and Sloan [14]. The main new ingredient is a Dyson-Phillips expansion which has already been applied by

Davies [10] in related contexts. Its use in this setting is motivated by Berthier-Gaveau [6], Carmona [8] and Simon [29]. The first authors proved some interesting inequalities derived from Martingale inequalities on path integrals, and then Carmona [8] and Simon [29] independently realized their significance in simplifying the proofs of Herbst-Sloan [14]. Since $H_0(if)$ is the generator of a drift process one could directly apply the proof of [6], but given the realization of Simon [29] that their results come from a kind of disguised Dyson-Phillips expansion, we will avoid path integrals and use purely L^p analysis.

In the following f denotes a complex function on R^n satisfying the Lipshitz condition

$$|f(x)-f(y)| \leqq a|x-y| \tag{6.3}$$

for all $x, y \in R^n$. Let $H_0 = -\Delta$ on R^n. Formally

$$H_0(if) = e^f(-\Delta)e^{-f}$$

generates a semigroup $\exp(-tH_0(if))$ which for $t>0$ is given by the kernel

$$(4\pi t)^{-n/2} \exp(f(x)-f(y)-|x-y|^2/4t). \tag{6.4}$$

In fact we can define $H_0(if)$ on L^q for $1 \leqq q \leqq \infty$ as the generator of the semigroup (6.4):

Lemma 6.1. *Let f obey* (6.3) *q and let* $\exp(-tH_0(if))$ *be defined by the kernel* (6.4) *for $0<t<\infty$. Then* (i) $\exp(+tH_0(if))$ *is a bounded operator from $L^p(R^n)$ to $L^q(R^n)$ for any pair p, q with $1 \leqq p \leqq q \leqq \infty$, with norm*

$$\|e^{-tH_0(if)}\|_{p,q} \leqq C_{p,q} t^{-r}$$

for $0<t<1$, where $r=(p^{-1}-q^{-1})n/2$.

(ii) $\exp(-tH_0(if)$ *is a strongly continuous semigroup on L^q for $1 \leqq q < \infty$.*

Proof. (i) By (6.3) the kernel (6.4) is bounded by $K_t^n(x-y)$ where

$$K_t^n(x) = (4\pi t)^{-n/2} \exp(a|x| - x^2/4t). \tag{6.5}$$

It follows from Young's inequality that

$$\|e^{-tH_0(if)}\|_{p,q} \leqq \|K_t^n(\cdot)\|_s$$

with $s^{-1} = 1 + q^{-1} - p^{-1}$. (i) follows from noting that as $t \to 0$

$$\|K_t^n(\cdot)\|_s = O(t^{-(1-s^{-1})n/2}). \tag{6.6}$$

(ii) $\exp(-tH_0)$ is a strongly continuous semigroup on $L^q(i \leqq q < \infty)$. For $f \neq 0$ the semigroup property is obvious from the definition. Strong continuity for $t \to 0$ follows from

$$\|e^{-tH_0(if)} - e^{-tH_0}\|_{q,q} = O(t^{1/2}).$$

This estimate is obtained from Young's inequality by noting that the kernal of $[\exp(-tH_0(if)) - \exp(-tH_0)]$ is bounded by $a|x-y|K_t^n(x-y)$. $\square$

Lemma 6.2. *Let $\tilde{W}$ be a function on R^n of the form $\tilde{W}(x) = W(y)$, where y is the orthogonal projection of x onto a v-dimensional subspace (denoted by R^v) of R^n. If*

$W \in L^p(R^\nu)$ for some $p > \nu/2$ and if f satisfies (6.3) *then*

$$\int_0^1 dt \| \tilde{W} e^{-tH_0(if)} \|_{q,q} < \infty$$

for all q in $1 \leqq q \leqq p$.

Remarks. In the application to Schrödinger operators, $\tilde{W}$ will be a pair- or multiparticle-potential. It is also possible to treat potentials which are only uniformly locally L^p (see [29]).

Proof. Representing $x=(x_1, x_2)$ by its components $x_1 \in R^\nu$ and $x_2 \perp R^\nu$ we obtain from (6.3)

$$|f(x)-f(y)| \leqq a|x_1-y_1| + a|x_2-y_2|$$

so that the kernel of $\tilde{W} \exp(-tH_0(if))$ is bounded by the function

$$|W(x_1)| K_t^\nu(x_1-y_1) K_t^{n-\nu}(x_2-y_2)$$

defined by (6.5). Using Hölder's and Young's inequalities one finds

$$\| \tilde{W} e^{-tH_0(if)} \|_{q,q} \leqq \| W \|_{sq} \| K_t^\nu(\cdot) \|_r \| K_t^{n-\nu}(\cdot) \|_1$$

for $1 \leqq s \leqq \infty$ and $r^{-1} = r - (sq)^{-1}$. Since $q \leqq p$ we may set $s = p/q$. Then $1 - r^{-1} = p^{-1}$ and by (6.6), as $t \to 0$:

$$\| K_t^\nu(\cdot) \|_r = O(t^{\nu/2p}); \quad \| K_t^{n-\nu}(\cdot) \|_1 = O(1). \quad \square$$

Lemma 6.3. *Let f obey* (6.3) *and let V be a finite sum of functions $\tilde{W}$ satisfying the hypothesis of Lemma 5.2. Then $P^t = \exp[-t(H_0(if)+V]$ is a bounded semigroup on L^q for $1 \leqq q \leqq \infty$.*

Remark. A constructive definition of $P^t$is given in the proof. The notation implies that the semigroups P^t on L^q and P^t on L^p coincide on $L^p \cap L^q$.

Proof. V is a closed operator on L^1 (on its natural domain) and

$$\int_0^1 \| V e^{-tH_0(if)} \|_{1,1} dt < \infty$$

by Lemma 6.1. Therefore $H_0(if)+V$ is the generator of a strongly continuous semigroup P^t on L^1 which can be constructed by the Dyson-Phillips expansion for sufficiently small $t > 0$:

$$P^t = \sum_{n=0}^{\infty} \int_{\substack{t_i \geqq 0 \\ t_0 + t_1 + \ldots + t_n = t}} dt_1 \ldots dt_n e^{-t_0 H_0(if)} V e^{-t_1 H_0(if)} \ldots V e^{-t_n H_0(if)}.$$

Next we note that $-\bar{f}$ also satisfies (6.3). Exhibiting the f-dependence of P^t we can therefore define

$$P^t(f) \equiv P^t(-\bar{f})^* \tag{6.7}$$

as a semigroup on L^∞. Using the Dyson-Phillips expansion one sees that the two definitions coincide on $L^1 \cap L^\infty$. By the Riesz-Thorin interpolation theorem [24]

$P^t(f)$ is defined as a semigroup on each $L^q(1 \leqq q \leqq \infty)$ with the bound

$$\|P^t(f)\|_{q,q} \leqq \|P^t(f)\|_{1,1}^{q} \|P^t(-\bar{f})\|_{1,1}^{1-q}. \quad \square \tag{6.8}$$

Remark. Another way of constructing P^t is the following: first, assume that V is a sum of functions $\tilde{W}$ satisfying the hypothesis of Lemma 6.2 with $W \in L^p(R^\nu) \cap L^\infty(R^\nu)$, $p > \nu/2$. Since $V \in L^\infty$, $P^t(f)$ can be defined on *all* L^q by the Dyson-Phillips expansion and satisfies (6.7) and (6.8). Noting that $\|P^t\|_{1,1}$ involves only the norms $\|W\|_p$ we can then define P^t in the general case as a uniform limit (on each L^q), by approximating each $W \in L^p(R^\nu)$ from $L^p(R^\nu) \cap L^\infty(R^\nu)$.

Lemma 6.4. *Let f be a real function satisfying* (6.3). *Then under the hypothesis of Lemma 6.3, P^t is bounded from L^2 to L^∞ for all $t > 0$.*

Proof. Let $t > 0$ and $P^t(\lambda) = \exp[-t(H_0(if) + \lambda V]$. Assuming first that $V \in L^\infty$, $P^t(\lambda)$ is an entire function of λ as can be seen from the Dyson-Phillips expansion. It satisfies the pointwise estimate

$$|P^t(\lambda)h| \leqq P^t(\mathrm{Re}\,\lambda)|h|$$

for $h \in L^2$, which follows from the Trotter product formula (see [13] or [14]). Hadamard's three line theorem [24] applied to the function $\varphi(z) = P^t(2z)|h|^{2-2z}$ gives

$$\|P^t(1)h\|_\infty \leqq \|P^t(2)1\|_\infty^{1/2} \|P^t(0)|h|^2\|_\infty^{1/2}.$$

Using Lemmas 6.1 and 6.3 we find

$$\|P^t(1)\|_{2,\infty} \leqq \|P^t(2)\|_{\infty,\infty}^{1/2} \cdot C_{1,\infty}^{1/2} t^{-n/8}.$$

By the approximation argument described above, this estimate extends to all V obeying the hypothesis of Lemma 6.3. $\square$

Proof of Theorem 1.3. First we remark that the operator sum $H_0(if) + V$ is the generator of the semigroup P^t on L^2. This follows from Lemma 6.2 where we may set $q = 2$ since $p \geqq 2$ by hypothesis, so that P^t is defined by the Dyson-Phillips expansion on L^2. It follows that $P^t = e^f(e^{-tH})e^{-f}$. Therefore, $H\psi = E\psi$ and $e^f\psi \in L^2$ imply $P^t e^f \psi = e^{-tE} e^f \psi$ for all $t > 0$. By Lemma 6.4, $P^t e^f \psi \in L^\infty$ for $t > 0$, hence $e^f \psi \in L^\infty$. $\square$

Theorem 6.1 (Ultimate COST estimate). *Under the hypothesis of Theorem 5.1 f is an L^∞ exponential bound.*

Proof. By Theorem 1.3 the regularizations f_j of f defined by (5.3) are L^∞ exponential bounds. From the argument following (5.4) one sees that f is an L^∞ exponential bound. $\square$

As a useful particular case we note:

Theorem 6.2. *Let $H\psi = E\psi$ where H is an N-particle Hamiltonian obeying* ($C3$). *Let $f_1 \ldots f_m$ be positive C^1-functions on $X \setminus \{0\}$ which are homogeneous of degree* 1. *Let $a_i = \nabla f_i$ and $S_i = \{x | f_i(x) \leqq f_k(x)$ for $k = 1 \ldots m\}$. Then*

$$f(x) = \min_i f_i(x)$$

is an L^∞ exponential bound for ψ if for each i

$$(\Pi_D a_i(x))^2 \leqq \Sigma_D - E$$

for all $x \in S_i \setminus \{0\}$ and all $D \rhd D(x)$.

Proof. For any fixed $x \neq 0$ let $J = \{i | x \in S_i\}$. Given $\varepsilon > 0$ there exists a neighbourhood N_x of x where $f_i > f$ for $i \notin J$ and $(1-\varepsilon)^2 (\Pi_D a_i)^2 \leqq \Sigma_D - E$ for $i \in J$ and all $D \rhd D(x)$. Therefore $(1-\varepsilon) f$ has the Lipschitz properties

$$(1-\varepsilon)|f(y) - f(z)| \leqq (\Sigma_D - E)^{1/2} |y - z|$$

for all $D \rhd D(x)$ and all $y, z \in N_x$ with $\Pi_D(y-z) = y - z$. It follows that $(1-\varepsilon) f$ has an L^∞ gradient obeying the hypothesis of Theorem 5.1. □

§ 7. Atomic Systems

In this section we construct explicit exponential bounds for a class of systems which includes "atoms" with infinite nuclear mass. In particular we will recover the bounds of [3, 4] except for the preexponential factors.

Definition. A *pseudo-atomic Hamiltonian* is an operator

$$H_N = \sum_{i=1}^{N} (p_i^2 + V(x_i)) + \sum_{i<k}^{1 \dots N} W(x_i - x_k)$$

on $L^2(R^{\nu N})$, with potentials V and W obeying the condition (C3) of § 1, and such that

$$K_N = \sum_{i=1}^{N} p_i^2 + \sum_{i<k}^{1 \dots N} W(x_i - x_a) \geqq 0 .$$

Remarks. Such a Hamiltonian describes a system of $N+1$ particles $0, 1 \dots N$: a "nucleus" 0 at $x_0 = 0$ and N "electrons" $1 \dots N$. It has three important properties:

(i) The mass of the nucleus is infinite.

(ii) The electrons are identical.

(iii) The energy of any subsystem consisting only of electrons is nonnegative, since $\sigma(K_n) \subset \sigma(K_N)$ for $n \leqq N$ by (3.5).

Each one of these properties drastically simplifies the task of constructing exponential bounds from Theorem 5.1. The kinematical simplifications due to (i) are described at the end of Appendix 1. By (ii) and (iii) the thresholds are the "ionization-thresholds"

$$\Sigma_D = E_n \equiv \inf \sigma(H_n) \qquad (n = 0, 1, \dots, N-1)$$

which only depend on the number n of electrons in the same cluster with the nucleus. They are ordered in the sense

$$E_{N-1} \leqq E_{N-2} \leqq \dots \leqq E_0 = 0 ,$$

since $\sigma(H_n) \subset \sigma(H_m)$ for $n \leqq m$ by (3.5). As a consequence of Lemma 1.2, the gradient conditions (5.1) or (5.2) need only hold for decompositions of the form D

$=(0i_1\dots i_n)(i_{n+1})(i_{n+2})\dots(i_N)\rhd D(x)$, which by (i) implies $x_{i_1}=\dots=x_{i_n}=0$. Finally, (ii) suggests that we try to construct exponential bounds $f(x_1\dots x_N)$ which are totally symmetric in $x_1\dots x_N$.

Theorem 7.1. *Let H_N be a pseudo-atomic Hamiltonian with the tresholds $E_{N-1}\leqq E_{N-2}\dots\leqq E_0=0$ and with an eigenvalue $E_N<E_{N-1}$. Let f be a positive C^1-function on the interior of the sector $S=\{r=(r_1\dots r_N)|0\leqq r_1\leqq r_2\dots\leqq r_N<\infty\}$ of R^N, which is homogeneous of degree 1 and for which f and its first derivatives are continuous up to the boundary of S (except $r=0$). Let F be the symmetric function on X equal to $f(|x_1|\dots|x_N|)$ on the sector $T=\{x|0\leqq|x_1|\leqq\dots\leqq|x_N|\}$. Then F is an L^∞ exponential bound for any ψ with $H\psi=E_N\psi$ if for each $n=0,1,\dots,N-1$*

$$\sum_{n+1}^{N}\left[\frac{\partial f}{\partial r_i}(r)\right]^2\leqq E_n-E_N \tag{7.1}$$

for all r with $0=r_1=\dots=r_n$.

Remark. It is easy to see that (7.1) is necessary for F to obey (5.2).

Proof. Given $\varepsilon>0$ we define the function f_ε on S by

$$f_\varepsilon(r)=f(\varrho),\quad\text{where}\quad \varrho_i=(\varepsilon^2r^2+r_i^2)^{1/2}.$$

Since f is positive and homogeneous of degree 1 and since $\varrho_i\geqq r_i$, we have $f_\varepsilon\geqq f$ on S and $F_\varepsilon\geqq F$ for the corresponding symmetric functions on X. Therefore F is an exponential bound if for any γ with $0<\gamma<1$, $(1-\gamma)F_\varepsilon$ satisfies the hypothesis of Theorem 6.3 for sufficiently small $\varepsilon=\varepsilon(\gamma)>0$.

At any interior point x of T we can compute the gradient $\nabla F_\varepsilon(x)$ by

$$\begin{aligned}(\nabla F_\varepsilon(x))_i&=\frac{\partial F_\varepsilon}{\partial x_i}(x)=\sum_k\frac{\partial f}{\partial r_k}(\varrho)\frac{\partial\varrho_k}{\partial x_i}\\&=x_i\sum_k\frac{\partial f}{\partial r_k}(\varrho)\varrho_k^{-1}(\delta_{ik}+\varepsilon^2),\end{aligned}\tag{7.2}$$

where $r_i=|x_i|$. If $\pi:(x_1\dots x_N)\to(x_{k_1}\dots x_{k_N})$ is a permutation acting on X, we then obtain ∇F_ε at the permuted point πx by

$$\nabla F_\varepsilon(\pi x)=\pi\nabla F_\varepsilon(x). \tag{7.3}$$

Thus we see that ∇F_ε is continuous on the interior of T (and of each permuted sector πT). Moreover, as we go from the interior to the boundary of T (or of πT), ∇F_ε has continuous boundary values for $x\neq 0$ which are still given by (7.2) (or (7.2) and (7.3)). Therefore ∇F_ε is a piecewise continuous function on X which in general takes several limiting values at points $x\neq 0$ on sector boundaries. In particular, for $x\in T\setminus\{0\}$, these values are $\{\pi\nabla F_\varepsilon(x)\}$ where $\nabla F_\varepsilon(x)$ is given by (7.2) and where π runs over all permutations obeying $\pi x=x$.

Since $(1-\gamma)F_\varepsilon$ is symmetric, it is sufficient to check (5.2) for $x\in T\setminus\{0\}$. In view of Theorem (1.2) and of the continuity properties of ∇F_ε we need only show that

$$(1-\gamma)^2(\Pi_D\pi\nabla F_\varepsilon(x))^2\leqq E_n-E_N$$

for all $D=(0,i,\dots,i_n)(i_{n+1})\dots(i_N)\rhd D(x)$ and all π with $\pi x=x$. Now $D\rhd D(x)$ and $x\in T$ imply $x_1=\dots=x_n=0$ and, by (7.2), $\partial F_\varepsilon/\partial x_1=\dots=\partial F_\varepsilon/\partial x_n=0$. (This is the motivation for introducing f_ε.) Since π is orthogonal and Π_D is a projection, it therefore suffices that

$$(1-\gamma)^2 \sum_{n+1}^{N} \left[\frac{\partial F_\varepsilon}{\partial x_i}(x)\right]^2 \leqq E_n - E_N \tag{7.4}$$

for each $n=0,1,\ldots,N-1$ and all $x\in T\setminus\{0\}$ with $x_1=\ldots=x_n=0$. Using $r_i\leqq\varrho_i$ and $\varrho_i\geqq\varepsilon|r|$ we obtain from (7.2):

$$\left|\frac{\partial F_\varepsilon}{\partial x_i}(x)\right| \leqq \left|\frac{\partial f}{\partial r_i}(\varrho)\right| + \varepsilon\sum_k \left|\frac{\partial f}{\partial r_k}(\varrho)\right|. \tag{7.5}$$

Since all terms are homogeneous of order 0, we may restrict x to $|x|=1$. Then $|\varrho_i - r_i|\leqq\varepsilon$, and since $\partial f/\partial r_i$ is uniformly continuous for $r\in S$, $|r|=1$, it follows that $(\partial f/\partial r_i)(\varrho)\to(\partial f/\partial r_i)(r)$ uniformly as $\varepsilon\to 0$. Moreover, for $n=0$, (7.1) gives the bound $|\partial f/\partial r_i|\leqq E_N$ for all r and we see that the right-hand side of (7.5) converges to $|(\partial f/\partial r_i)(r)|$ uniformly in $r\neq 0$ as $\varepsilon\to 0$. By (7.1) we can therefore choose $\varepsilon>0$ so that (7.4) holds. □

Example 7.1. $f=(r_1^2+\ldots+r_N^2)^{1/2}(E_{N-1}-E_N)^{1/2}$. This is O'Connor's bound: $F(x) = |x|(E_{N-1}-E_N)^{1/2}$ which is always the best *isotropic* bound.

Example 7.2. $f=r_1(E_0-E_1)^{1/2}+r_2(E_1-E_2)^{1/2}+\ldots r_N(E_{N-1}-E_N)^{1/2}$. This coincides with example 7.1 if $r_1=\ldots=r_{N-1}=0$. For all other r, f is larger than O'Connors bound if the successive ionisation potentials are increasing, i.e. if

$$E_{N-1}-E_N\leqq E_{N-2}-E_{N-1}\leqq\ldots\leqq E_0-E_1, \tag{7.6}$$

which is an *experimental* fact for "real" atoms. Presumably, f is then the optimal bound allowed by Theorem 6.3. Assuming (7.6), Alrichs and M. and T. Hoffmann-Ostenhof [4] have recently derived the same exponential bound by subharmonic comparison methods.

Example 7.3. $f_k=(E_k-E_N)^{1/2}\left(\sum_{k+1}^{N} r_i^{-1}\right)^{-1}$ $k=0,1,\ldots,N-1$. This is seen to obey (7.1) except for a lack of continuity of ∇f_k as several r_i go to zero. However, (7.1) holds for any limiting value and the proof of Theorem 7.1 can be adapted to cover this case. This is the basic estimate in [3].

In the following examples we show how to improve the bound of example 7.2 in the case where (7.6) does not hold. While this is of no interest for real atoms, it prepares the ground for general 3-body systems (§8).

Example 7.4. ($N=2$) We start with the 2 functions

$$f_{(1)(2)}=r_1(E_0-E_1)^{1/2}+r_2(E_1-E_2)^{1/2}$$
$$f_{(12)}=(r_1^2+r_2^2)^{1/2}(E_0-E_2)^{1/2},$$

which by the Schwarz inequality satisfy $f_{(1)(2)}\leqq f_{(12)}$ for all r_1,r_2 and coincide for $r_1^2(E_1-E_2)=r_2^2(E_0-E_1)$. On this set not only the 2 functions but also their gradients take the same values, since a non-negative C^1-function has vanishing first derivatives at its zeros. Defining f piecewise by

$$f = f_{(1)(2)} \quad \text{if} \quad r_2^2(E_0 - E_1) \geqq r_1^2(E_1 - E_2)$$

$$f = f_{(12)} \quad \text{otherwise},$$

we therefore obtain a C^1-function of (r_1, r_2), the "Mercuriev function" of Example 2.3. Both its pieces saturate the gradient condition $\alpha_1^2 + \alpha_2^2 \leqq E_0 - E_2$ for all r_1, r_2. The subset $r_1 = 0$ is in the domain of $f_{(1)(2)}$, which also saturates $\alpha_2^2 \leqq E_1 - E_2$. The situation is shown in Fig. 2:

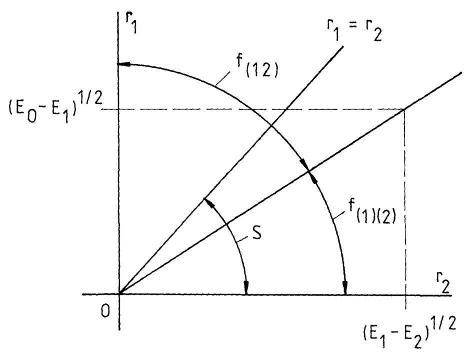


Fig. 2

Only the restriction of f to the sector S is relevant as an exponential bound. We see that $f = f_{(1)(2)}$ on all of S if and only if $E_1 - E_2 \leqq E_0 - E_1$, so that in this case we have not improved the estimate given in example 7.2. In any case, the minimal exponential fall-off is in the 2-direction and coincides with O'Connors bound.

Example 7.5. $(N = 3)$ We start with the 4 functions

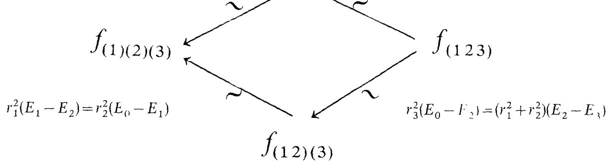
$$f_{(1)(2)(3)} = r_1(E_0 - E_1)^{1/2} + r_2(E_1 - E_2)^{1/2} + r_3(E_2 - E_3)^{1/2}$$

$$f_{(1)(23)} = r_1(E_0 - E_1)^{1/2} + (r_2^2 + r_3^2)^{1/2}(E_1 - E_3)^{1/2}$$

$$f_{(12)(3)} = (r_1^2 + r_2^2)^{1/2}(E_0 - E_2)^{1/2} + r_3(E_2 - E_3)^{1/2}$$

$$f_{(123)} = (r_1^2 + r_2^2 + r_3^2)^{1/2}(E_0 - E_3)^{1/2}$$

The partial order among these functions and the sets where two (ordered) functions coincide can easily be read off by the Schwarz inequality:



(7.7)

Here the arrows go in the decreasing direction, and attached to them are the manifolds where the 2 functions coincide. These 4 manifolds intersect on the ray R

defined by

$$r_1^2 : r_2^2 : r_3^2 = E_0 - E_1 : E_1 - E_2 : E_2 - E_3 ,$$

where $f_{(1)(2)(3)} = f_{(123)}$. It is now easy to cut $(R^+)^3$ into 4 cones on each of which f can be defined by one of the 4 pieces:

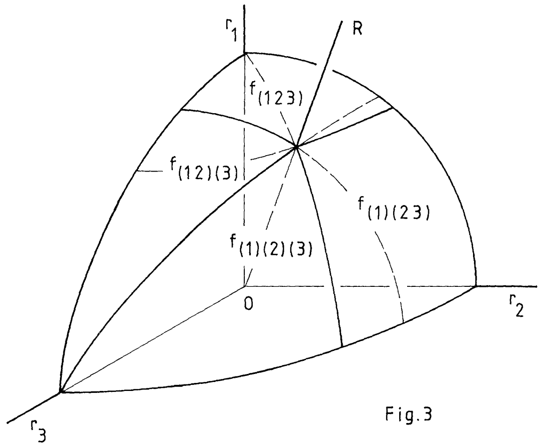


Fig. 3

On the unit sphere, the domain of $f_{(1)(2)(3)}$ is bounded by great circles and the domain of $f_{(123)}$ by circles parallel to the 12- and 23-planes. The inequalities which define the 4 sectors are easily written down from the diagram (7.7). For example we have $f = f_{(1)(2)(3)}$ if

$$\begin{aligned} &r_3^2(E_1 - E_2) \geqq r_2^2(E_2 - E_3) \quad \text{and} \\ &r_2^2(E_0 - E_1) \geqq r_1^2(E_1 - E_2) . \end{aligned} \tag{7.8}$$

From this one can show that the minimum of the piece $f_{(1)(2)(3)}$ (on the unit sphere) is in the 3-direction. This is also the minimum of f, since the other pieces take all their values on the boundary with $f_{(1)(2)(3)}$. Hence we have again

$$f(x) \geqq |x|(E_2 - E_3)^{1/2} ,$$

exhibiting O'Connors bound. By the same argument as for $N=2$, f is a C^1-function of $r_1 \dots r_3$ and it is easily checked that all gradient conditions are saturated.

Again it is only the restriction of f to the sector $S: 0 \leqq r_1 \leqq r_2 \leqq r_3$ which gives the exponential bound. On the unit sphere, S is bounded by great circles just as the domain of $f_{(1)(2)(3)}$, but (instead of R) with respect to the ray $R_S : r_1 = r_2 = r_3$. Therefore it depends on the ratios of the numbers $E_n - E_{n-1}$ which of the 4 pieces of f participate in the exponential bound. In particular, $f = f_{(1)(2)(3)}$ on all of S if and only if the ray R_S is in the domain (7.8), i.e. if and only if

$$E_2 - E_3 \leqq E_1 - E_2 \leqq E_0 - E_1 .$$

In the general N-electron case, f must be pieced together from the functions

$$f_D = (r_1^2 + \dots + r_n^2)^{1/2}(E_0 - E_n)^{1/2} + \dots + (r_{m+1}^2 + \dots + r_N^2)^{1/2}(E_m - E_N)^{1/2} ,$$

where $D=(1 \dots n) \dots (m+1 \dots N)$ is any order-preserving partition of $(1 \dots N)$. If the ionisation potentials obey (7.6) f reduces to the bound given in example 7.2.

§8. General 3-Body Systems

We try to extend the procedure used in the atomic case as follows: let $S=(D_1 \dots D_N)$ be a given string (see Appendix 1) and let

$$E \equiv \Sigma_1 < \Sigma_2 \leqq \dots \leqq \Sigma_N = 0$$

be the corresponding sequence of thresholds including the energy of the bound state. As candidates for exponential bounds we consider positive, homogeneous C^1-functions $f(r_2 \dots r_N)$ of the variables $r_m = |\Delta_m x|$ (Jacobi coordinates associated with the string S). Setting $\alpha_m = \partial f / \partial r_m$, the gradient of $f(x)$ as a function on X is

$$a(x) = \sum_{m=2}^{N} \alpha_m \Delta_m x / r_m ,$$

and since $\Pi_n = \Delta_2 + \dots + \Delta_n$,

$$(\Pi_n a)^2 = \sum_{m=2}^{n} \alpha_m^2 .$$

Therefore f satisfies the gradient conditions for *all* $D \in S$ provided that

$$\alpha_2^2 + \dots + \alpha_n^2 \leqq \Sigma_n - \Sigma_1$$

for $r_{n+1} = \dots = r_N = 0$, and all $n = 2 \dots N$.

The problem of finding the largest possible f_S compatible with these conditions is the same as in the atomic case. Having solved it for all strings S, the question is still open how to construct from the functions f_S an exponential bound which satisfies the gradient conditions *for all* D.

Example 5 ($N=3$). There are 3 strings $S=(D_1 D_2 D_3)$, given by the 3 possible decompositions D_2. Rewriting example 7.4 in the present notation, we have

$$f_S = r_2(\Sigma_2 - \Sigma_1)^{1/2} + r_3(\Sigma_3 - \Sigma_2)^{1/2}$$

if $r_2^2(\Sigma_3 - \Sigma_2) \geqq r_3^2(\Sigma_2 - \Sigma_1)$,

$$f_S = (r_2^2 + r_3^2)^{1/2} (\Sigma_3 - \Sigma_1)^{1/2}$$

otherwise.

Clearly, this satisfies the gradient conditions for D_3 (all x) and D_2 ($x_3 = 0$). Now let S' be a second string. The relation between the 2 sets of Jacobi coordinates can be visualised as follows:

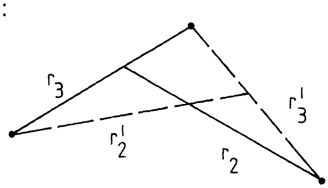


Fig. 4

Here the r's are proportional to the distances shown in the figure with factors depending only on the masses. In general, r'_2 and r'_3 cannot be expressed as functions of r_2 and r_3 alone and f_S cannot easily be compared with $f_{S'}$. However, if $r'_3=0$, we have (with $r=|x|$):

$$r'_2=r; \quad r_2=\beta_2 r; \quad r_3=\beta_3 r;$$

with constants β_2, β_3 depending only on the masses. On the 3-dimensional plane $R'_2=$range of $\Pi_{D'_2}$ both f_S and $f_{S'}$ therefore reduce to isotropic functions:

$$f_S=r\beta$$

$$f_{S'}=r(\Sigma'_2-E)^{1/2}$$

and we see that f_S satisfies the gradient condition for D'_2 if and only if $f_S(x)\leqq f_{S'}(x)$ for one point $x\in R'_2$, $x\neq 0$. Stated more generally, f_S satisfies the gradient conditions imposed on $f_{S'}$ on the set $\{x|f_S(x)\leqq f_{S'}(x)\}$. Using Theorem 6.2, we conclude:

Theorem 8.1. *Let H be a 3-particle Hamiltonian obeying (C.3) and let f_S be the function defined in Example 5. Then $f(x)=\min_S f_S(x)$ is an L^∞-exponential bound or, equivalently,*

$$|\psi(x)|\leqq C(\varkappa)\sum_S e^{-\varkappa f_S(x)}$$

with $C(\varkappa)<\infty$ for $\varkappa<1$.

From the construction it is difficult to judge whether this bound is optimal or not. It is, however, in full agreement with Mercuriev's results on the asymptotic behaviour of bound state wave functions [21]. Using the Faddeev equations (for short range potentials) he obtains

$$\psi(x)=\sum_S \psi_S(x)$$

and an exponential fall-off of $\psi_S(x)$ precisely given by $f_S(x)$.

Appendix 1. N-Particle Systems in the CM-Frame

In this appendix we present a compact formalism for N-particle kinematics. The configuration space of N mass points m_i with cartesian coordinates $x^i\in R^\nu$ and with fixed center of mass at the origin of R^ν is

$$X=\left\{x=(x^1\dots x^N)\,\middle|\,\sum_{i=1}^N m_i x^i=0\right\}.$$

It has the dimension $n=\nu(N-1)$ and is equipped with the scalar product

$$(x,y)\equiv 2\sum_{i=1}^N m_i x^i y^i, \tag{A1.1}$$

where $x^i y^i$ is the scalar product in R^ν. We will also use the notation $x^2=(x,x)$ and $|x|=(x,x)^{1/2}$. The length $R(x)$ defined by $x^2=2mR^2$ (m = total mass) is the radius of gyration.

$\bar{X}$ denotes the complexification of the real space X (i.e. $x^i \in C^\nu$ for $x \in \bar{X}$) and we denote with (x,y) the *bilinear* form on $\bar{X}$ which reduces to (A1.1) for real x, y.

Using the scalar product (A1.1) we *identify* X *with its dual*: $k \in X$ is identified with the linear form

$$x \to (k,x) \equiv \sum_{i=1}^{N} k_i x^i,$$

where the covariant coordinates $k_i \in R^\nu$ are uniquely defined by the condition $\sum k_i = 0$, and given by $k_i = 2m_i k^i$. In particular the classical particle momenta p_i are the covariant coordinates of the vector $p = 1/2(dx/dt)$ and p^2 is the kinetic energy.

The volume element of X is defined by the metric (A1.1) and $\mathscr{H} = L^2(X)$ is the Hilbert space of the quantum mechanical N-particle system with fixed center of mass. The transition to the momentum representation is the usual one:

$$\psi(x) = (2\pi)^{-n/2} \int_X dk \hat{\psi}(k) e^{i(k,x)}$$

$$\hat{\psi}(k) = (2\pi)^{-n/2} \int_X dx \psi(x) e^{-i(k,x)}.$$

Expressed in terms of the covariant coordinates, $\hat{\psi}(k_1, \dots k_N)$ is defined on the set $\sum k_i = 0$ and the particle momenta are described by the operators

$$p_i : \hat{\psi}(k) \to k_i \hat{\psi}(k)$$

obeying the operator identity $\sum p_i = 0$. They are the covariant components of the vector operator p generating the unitary group of translations

$$U(a) = e^{-i(p,a)} : \psi(x) \to \psi(x-a) \qquad (a \in X).$$

For smooth ψ, $(ip\psi)(x) = (\nabla\psi)(x) \in \bar{X}$ is the gradient of ψ at the point x.

The N-particle Hamiltonian in the CM-frame is

$$H = \sum p_i^2 (2m_i)^{-1} + V = p^2 + V = H_0 + V,$$

where V is assumed to be a sum of local 2-body potentials:

$$V(x) = \sum_{i<k} V_{ik}(x^i - x^k).$$

Let C be a subset (cluster) of particles and $x_C \in R^\nu$ its center of mass:

$$x_C = m_C^{-1} \sum_{i \in C} m_i x^i; \qquad m_C = \sum_{i \in C} m_i.$$

We define the linear operator Π_C on X by

$$(\Pi_C x)^i = \begin{cases} x^i - x_C & \text{if} \quad i \in C, \\ 0 & \text{otherwise}. \end{cases}$$

Since $\Pi_C^2 = \Pi_C$ and $(x, \Pi_C y) = (\Pi_C x, y)$, Π_C is an orthogonal projection. It acts on the (covariant) particle momenta as follows:

$$(\Pi_C p)_i = \begin{cases} p_i - m_i p_C / m_C & \text{if} \quad i \in C, \\ 0 & \text{otherwise}, \end{cases}$$

where $p_C = \sum p_i$ $(i \in C)$ is the total momentum of the cluster C. Note that $(\Pi_C p)^2$ is the kinetic energy of the cluster C in its own CM-frame.

Let $D = (C_1 \dots C_m)$ be a partition of $(1 \dots N)$ into clusters. Then the projections Π_C for $C \in D$ are mutually orthogonal and

$$\Pi_D \equiv 1 - \sum_{C \in D} \Pi_C \tag{A1.2}$$

is again a projection and orthogonal to all Π_C for $C \in D$. It acts as

$$(\Pi_D x)^i = x_C; \qquad (\Pi_D p)_i = m_i p_C / m_C,$$

where C is the cluster containing particle i. In particular

$$(\Pi_D p)^2 = \sum_{C \in D} p_C^2 / 2m_C$$

is the kinetic energy of the intercluster motion and the relation

$$p^2 = (\Pi_D p)^2 + \sum_{C \in D} (\Pi_C p)^2$$

obtained from (A1.2) expresses the fact that the total kinetic energy is the sum of the internal kinetic energies of the clusters and of the intercluster kinetic energy. Correspondingly, the vectors $\Pi_C x$ describe the configurations inside the clusters $C \in D$ and $\Pi_D x$ the configuration of the centers of mass of the clusters. Both together determine the N-particle configuration

$$x = \Pi_D x + \sum_{C \in D} \Pi_C x .$$

For $D = (C_1 \dots C_m)$ let X_C $(C \in D)$ and X_D be the mutually orthogonal ranges of the operators Π_C and Π_D, respectively. Then

$$X = X_D \oplus X_{C_1} \oplus \dots \oplus X_{C_m},$$

so that $\mathscr{H} = L^2(X)$ factors accordingly into

$$\mathscr{H} = \mathscr{H}_D \otimes \mathscr{H}_{C_1} \otimes \dots \otimes \mathscr{H}_{C_m}, \tag{A1.3}$$

where the factors are the L^2 spaces over the corresponding subspaces of X (if C contains only one particle, $X_C = \{0\}$ and $\dim \mathscr{H}_C = 1$). The operator

$$H_D = H - \text{(all pair-potentials linking different clusters)}$$

describes a system of non-interacting clusters. With respect to the factorisation (A1.3) it has the structure

$$\begin{aligned} H_D = {} & H_D^0 \otimes 1 \otimes \dots \otimes 1 \\ & + 1 \otimes H_{C_1} \otimes \dots \otimes 1 \\ & + \dots \\ & + 1 \otimes 1 \otimes \dots \otimes H_{C_m} \end{aligned} \tag{A1.4}$$

for which we simply write

$$H_D = H_D^0 + \sum_{C \in D} H_C .$$

Here H_C is the Hamiltonian of the cluster C in its own CM-frame and $H_D^0 = (\Pi_D p)^2$ the kinetic energy of the intercluster motion. If D is not the trivial decomposition into one cluster, this operator has the purely continuous spectrum $[0, \infty)$ and the spectrum of H_D is

$$\sigma(H_D) = \left[\Sigma_D \equiv \inf \sum_{C \in D} \sigma(H_C), \infty\right).$$

Σ_D is the threshold for the break-up process $(1 \dots N) \to (C_1) \dots (C_m)$.

The cluster decompositions D are partially ordered by the relation

$$D \lhd D'$$

expressing that each cluster of D' is contained in a single cluster of D. This is equivalent to the relation

$$\Pi_D \leqq \Pi_{D'} \tag{A1.5}$$

for the corresponding projections and has the consequence that

$$\Sigma_D \leqq \Sigma_{D'} . \tag{A1.6}$$

A *string* $S = (D_1 D_2 \dots D_N)$ is defined as a sequence of decompositions D_m into m clusters such that $D_m \lhd D_{m+1}$. D_1 is the trivial decomposition and D_N the decomposition into N single particles. The corresponding projections $\Pi_m \equiv \Pi_{D_m}$ satisfy

$$0 = \Pi_1 < \Pi_2 < \dots < \Pi_N = 1$$

so that the differences

$$\Delta_m \equiv \Pi_m - \Pi_{m-1} \qquad (m = 2 \dots N)$$

form a complete set of mutually orthogonal ν-dimensional projections. To see the significance of Δ_m, let C_1 and C_2 be the two clusters of D_m which are united to form the cluster $C = C_1 \cup C_2$ of D_{m-1}. Then

$$(\Delta_m x)^i = \begin{cases} x_{C_1} - x_C & \text{if} \quad i \in C_1 , \\ x_{C_2} - x_C & \text{if} \quad i \in C_2 , \\ 0 \quad \text{otherwise} , \end{cases}$$

and

$$(\Delta_m x)^2 = 2 m_C^{-1} m_{C_1} m_{C_2} (x_{C_1} - x_{C_2})^2 .$$

We see that there is a one-to-one correspondence between $\Delta_m x$ and the vector $y_m = x_{C_1} - x_{C_2} \in R^\nu$. In this sense the splitting

$$x = \sum_{m=2}^{N} \Delta_m x$$

amounts to the introduction of the Jacobi coordinates $y=(y_2 \dots y_N)\in R^{\nu(N-1)}$ associated with the string S.

To describe the "pseudo-atomic systems" in §7, we introduce an additional particle $i=0$ and let $m_0=\infty$ ("nucleus"). For the other particles ("electrons") we set $m_1=\dots=m_N=\frac{1}{2}$. Then the configuration space is

$$X=\{x=(x^0 \dots x^N)|x^0=0\}$$

and we can use $x^1 \dots x^N$ as *independent* coordinates, in which the metric is simply

$$(x,x)=\sum_{i=1}^{N}(x^i)^2.$$

Consequently, $x_i=x^i$ ($x_0=0$ by definition), and we may use lower indices throughout. Note, however, that clusters are subsets of $(0 \dots N)$ and that

$(\Pi_C x)_i=x_i$ if C contains the nucleus 0, and

$(\Pi_D x)_i=0$ if i is in the same cluster with the nucleus 0.

Appendix 2. Identical Particles

In this appendix we briefly indicate the few modifications necessary in the presence of identical particles, when the Hilbert-space $\mathscr{H}=L^2(X)$ is restricted to the corresponding symmetry sector $\mathscr{H}^S$. In §4, *$f(x)$ is assumed to be invariant under permutations of identical particles.* Then, instead of a single unit vector $e\in\Omega$ one always has to consider the equivalence class $\{e_i\}$ generated from e by permutations, the union of the corresponding cones $K_\varepsilon(e_i)$ and Weyl sequences in $C_0^\infty\cap\mathscr{H}^S$ with support in this union. Let $D(e)=(C_1 \dots C_m)$. Then by definition of $D(e)$, e is invariant under permutations *inside* the clusters and the same is true for $a(e)=\nabla f(e)$. The operator

$$H_D(a)=H_D^0(a_D)+\sum_{C\in D}H_C(a_C)$$

for $D=D(e)$ is therefore well defined on the bigger Hilbert-space

$$\mathscr{H}_D\otimes\mathscr{H}_{C_1}^S\otimes\dots\otimes\mathscr{H}_{C_m}^S \tag{A2.1}$$

where $\mathscr{H}_C^S$ is the allowed symmetry sector for the subsystem C, i.e. the space for the restriction of the representation of full permutation group to the subgroup of permutations within C. Redefining Σ_D as the infimum of $\sigma(H_D)$ on the space (A2.1), Theorem 4.1 and all its consequences remain formally unchanged. *As a rule, therefore, the conditions for exponential bounds are the same, with the understanding that only the thresholds of the correct symmetry type appear.*

Appendix 3. An Alternative Method of Geometric Spectral Analysis

In this appendix we discuss an alternative to the methods of §§3–4, which follows Simon's version [28] of Enss' proof [12]. It falls short of proving the basic result on $\sigma_{ess}(H(f))$ (Theorem 4.1) and thus has no application in the present context. However, it has some advantages in discussing invariant subspaces of H (as in the case of symmetries) and it can be used, for example, to delimit the essential spectrum of $H(\Theta)$ in dilation analytic theory or of $H(a)$ in the Combes-Thomas theory [9].

In the notation of §3 the basic identity used in [28] is

$$f(H)=f(H)X_0^n+\sum_D[f(H)-f(H_D)]X_D^n+\sum_D f(H_D)X_D^n, \tag{A3.1}$$

where D runs over all 2-cluster decompositions and where $\{X_0, X_D\}$ is the partition of unity introduced at the end of §3. Simon's argument proceeds from (A3.1) as follows: If $f\in C_0^\infty(R)$ the first term on the right is compact and the second term goes to zero in norm as $n\to\infty$. (This is proved for $f(x)=(x-i)^{-1}$ by commutator estimates as in §3 and then extended to all $f\in C_0^\infty(R)$ by an approximation argument.) If $\operatorname{supp} f\subset(-\infty,\Sigma)$, where Σ is the lowest threshold of H, then the last term in (A3.1) is zero and it follows that $f(H)$ is compact. A general argument then implies that $\sigma_{ess}(H)\subset[\Sigma,+\infty)$.

The above sketch depends heavily on the functional calculus for normal operators. Here we want to extend the arguments to non-normal H.

Theorem A3.1. *On a Banach space B let H, $\{H_i\}$, $i=1\ldots s$, be a family of closed operators and $\{X_i^n\}i=1\ldots s$, $1\leq n<\infty$ a family of uniformly bounded operators. Let*

$$X_0=1-\sum_{i=1}^{s}X_i^1$$

and suppose that

(i) $X_0(H-z)^{-1}$ *is compact for* $z\notin\sigma(H)$.

(ii) $(X_i^1-X_i^n)(H-x)^{-1}$ *and* $(X_i^1-X_i^n)(H_i-x)^{-1}$ *are compact for all n and all*

$$x\in\varrho\equiv\varrho(H)\cap\bigcap_{i=1}^{s}\varrho(H_i).$$

(iii) $\lim_{n\to\infty}\|X_i^n[(H-x)^{-1}-(H_i-x)^{-1}]\|=0.$ *for* $x\in\varrho$.

Then any connected component A of $\bigcap_i\varrho(H_i)$ is either entirely contained in $\sigma(H)$ or entirely disjoint from $\sigma_{ess}(H)$.

Remark. Using the X's introduced at the end of §3 one sees that $\sigma_{ess}(H)\subset\bigcup_c\sigma(H_c)$ for an N particle Hamiltonian with *complex* potentials.

Proof. Let $w\in A$ and suppose that $A\cap\varrho(H)\neq\Phi$. Pick $z_0\in\varrho$ and let $K=(H-z_0)^{-1}$, $K_i=(H_i-z_0)^{-1}$. Then for $|z|$ sufficiently large, z is in the resolvent sets of K and K_i and

$$(K-z)^{-1}=-z^{-1}-z^{-2}(H-(z_0+z^{-1})^{-1})^{-1} \tag{A3.2}$$

and similarly for K_i. From the identity

$$(H-z)^{-1}=X_0(H-z)^{-1}+\sum_i X_i^1(H_i-z)^{-1}$$
$$+\sum_i (X_i^1-X_i^n)[(H-z)^{-1}-(H_i-z)^{-1}]$$
$$+\sum_i X_i^n(H_i-z)^{-1}$$

we conclude by hypothesis that

$$(H-z)^{-1}=\sum_i X_i^1(H_i-z)^{-1}+\text{compact}.$$

Therefore, using (A3.2),

$$(K-z)^{-1}=-X_0 z^{-1}+\sum_i X_i^1(K_i-z)^{-1}+\text{compact}$$

for z sufficiently large. It follows that for any entire function f

$$f(K)=\sum_i X_i^1 f(K_i)+X_0 f(0)+\text{compact}. \qquad \text{(A3.3)}$$

Let $z_1=(w-z_0)^{-1}$. By the spectral mapping theorem z_1 is in the unbounded connected component of

$$\{z|z\neq 0, z\in\varrho(K_i) \quad \text{for} \quad i=1\ldots s\}.$$

By Runge's theorem there exists an entire function g with

$$u\equiv \sup_{z\in\{0\}\cup\bigcup_i \sigma(l_i)} < g(z_1)\equiv u+\varepsilon.$$

It follows from the spectral radius formula that

$$\lim_{m\to\infty} \|g^m(K_i)\|^{1/m}\leqq u,$$

so we can find m such that

$$\|g^m(K_i)\|\leqq(u+\tfrac{1}{2}\varepsilon)^m\left(\|X_0\|+\sum_i\|X_i^1\|\right)^{-1}$$

for all i. Let $f=g^m$ and note that

$$\left\|\left(X_0 f(0)+\sum_i X_i^1 f(K_i)\right)\varphi\right\|$$
$$\leqq \max\{|f(0)|, \|f(K_i)\|\}\left(\|X_0\|+\sum_i\|X_i^1\|\right)\|\varphi\|$$
$$<f(z_1)\|\varphi\|.$$

It follows that $\sum_i X_i^1 f(K_i)+X_0 f(0)$ has norm strictly less than $f(z_1)$ and so, by (A3.3) and Weyl's theorem on the invariance of the essential spectrum under compact perturbations (see e.g. [25], $f(z_1) \notin \sigma_{\text{ess}}(K)$. Thus, by the spectral mapping theorem, $w \notin \sigma_{\text{ess}}(H)$. □

References

1. Aguilar, J., Combes, J.M.: A class of analytic perturbations for one-body Schrödinger Hamiltonians. Commun. math. Phys. **22**, 269–279 (1971)
2. Alrichs, R.: Asymptotic behavior of atomic bound state wave functions. J. Math. Phys. **14**, 1860–1863 (1973)
3. Alrichs, R., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T.: Bounds for the long range behaviour of electronic wave functions. J. Chem. Phys. **68**, 1402–1410 (1978)
4. Alrichs, R., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T.: "Schrödinger inequalities" and asymptotic behaviour of many electron densities. Phys. Rev. (to appear)
5. Balslev, E., Combes, J.M.: Spectral properties of many-body Schrödinger operators with dilation analytic interactions. Commun. math. Phys. **22**, 280–294 (1971)
6. Berthier, A., Gaveau, B.: Critère de convergence des fonctionelles de Kac et application en mécanique quantique et en géometrie. J. Func. Anal. (to appear)
7. Brown, A., Pearcy, C.: Spectra of tensor products of operators. Proc. Am. Math. Soc. **17**, 162–166 (1966)
8. Carmona, A.: Marseille-Luminy preprints (in preparation)
9. Combes, J.M., Thomas, L.: Asymptotic behavior of eigenfunctions for multiparticle Schrödinger operators. Commun. math. Phys. **34**, 251–270 (1973)
10. Davies, E.B.: Properties of Green's functions of some Schrödinger operators. J. Lond. Math. Soc. **7**, 473–491 (1973)
11. Deift, P., Simon, B.: A time dependent approach to the completeness of multiparticle quantum systems. Comm. Pure Appl. Math. **30**, 573–583 (1977)
12. Enss, V.: A note on Hunzikers theorem. Commun. math. Phys. **52**, 233–238 (1977)
13. Guerra, F., Rosen, L., Simon, B.: The vacuum energy for $P(\phi)_2$. Infinite volume limit and coupling constant dependence. Commun. math. Phys. **29**, 233–247 (1973)
14. Herbst, I., Sloan, A.: Perturbation of translation invariant positivity preserving semigroups on $L^2(R^N)$. Trans. Am. Math. Soc. (to appear)
15. Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T.: "Schrödinger inequalities" and asymptotic behavior of the electron density of atoms and molecules. Phys. Rev. **16**A, 1782–1785 (1977)
16. Hunziker, W.: Space-time behavior of Schrödinger wave functions. J. Math. Phys. **7**, 300–304 (1966)
17. Jörgens, K., Weidmann, J.: Spectral properties of Hamiltonian operators. Lecture notes in mathematics, Vol. 319. Berlin, Heidelberg, New York: Springer 1973
18. Kato, T.: Perturbation theory for linear operators. Berlin, Heidelberg, New York: Springer 1966
19. Kato, T.: Schrödinger operators with singular potentials. Is. J. Math. **13**, 135–148 (1973)
20. Lavine, R.: Private communication
21. Mercuriev, S.P.: On the asymptotic form of three-particle wave functions of the discrete spectrum. Soviet J. Nucl. Phys. **19**, 222–229 (1974)
22. Morgan III, J.: The exponential decay of sub-continuum wave functions of two-electron atoms. J. Phys. A**10**, L91–L93 (1977)
23. O'Connor, T.: Exponential decay of bound state wave functions. Commun. math. Phys. **32**, 319–340 (1973)
24. Reed, M., Simon, B.: Methods of modern mathematical physics. II. Fourier analysis, self-adjointness. New York: Academic Press 1975
25. Reed, M., Simon, B.: Methods of modern mathematical physics. IV. Analysis of operators. New York: Academic Press 1978
26. Simon, B.: Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems. I. Proc. Am. Math. Soc. **42**, 395–401 (1974)
27. Simon, B.: Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems. III. Trans. Am. Math. Soc. **208**, 317–329 (1975)
28. Simon, B.: Geometric methods in multiparticle quantum systems. Commun. math. Phys. **55**, 259–274 (1977)

29. Simon, B.: Functional integration and quantum physics. New York: Academic Press (expected 1979)
30. Slaggie, E. L., Wichmann, E. H.: Asymptotic properties of the wave function for a bound nonrelativistic system. J. Math. Phys. **3**, 946–968 (1962)
31. Vock, E.: ETH thesis (in preparation)
32. Zhislin, G.: Discussion of the spectrum of the Schrödinger operator for systems of many particles. Tr. Mosk. Mat. Obs. **9**, 81–128 (1960)

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