

POINTWISE BOUNDS ON EIGENFUNCTIONS AND WAVE PACKETS IN N -BODY QUANTUM SYSTEMS. I

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ABSTRACT. We provide a simple proof of (a modification of) Kato's theorem on the Hölder continuity of wave packets in N -body quantum systems. Using this method of proof and recent results of O'Connor, we prove a pointwise bound

$$|\Psi(\zeta)| \leq D_\epsilon \exp[-(1 - \epsilon)a_0 |x|]$$

on discrete eigenfunctions of energy E . Here $\epsilon > 0$, $a_0^2 = 2$ (mass of the system) [$\text{dist}(E, \sigma_{\text{ess}})$] and $|x|$ is the radius of gyration.

1. Introduction. In 1957, T. Kato published a beautiful paper [2] which has not received the attention it deserves. Our secondary goal in this note is to provide a simple proof of Kato's result on the Hölder continuity of "wave packets" (i.e. vectors in $C^\infty(H)$) for N -body quantum systems on \mathbb{R}^{3N-3} with two body potentials. Our proof of this fact, which appears in §2, uses the basic elements of Kato's proof, especially an L^p -bootstrap; but by working in momentum space instead of configuration space, we avoid the use of modified fundamental solutions and the only L^p estimates we will need are Hölder's and Young's inequalities.

Our interest in Kato's paper was aroused by, and our major goal is related to, recent work of R. Ahlrichs [1] on the exponential falloff of discrete eigenfunctions of atomic systems. On physical grounds, one expects such an eigenfunction Ψ to behave more or less like $\exp(-a_0|x|)$ as $|x| \rightarrow \infty$ where $|x|$ is the radius of gyration of the system (see §3) and where a_0 is a simple function of the masses of particles and the distance of the eigenvalue from the essential spectrum, (see §3 for an explicit formula). Ahlrichs proves that $\exp(a|x|)\Psi \in L^2$ for any $a < a_0$. He then uses Kato's result to prove that Ψ obeys a pointwise bound

$$(1) \quad |\Psi(x)| \leq C_b \exp(-b|x|)$$

where $b < \alpha a_0$ with α an explicit constant smaller than 1. One expects a bound of the form (1) to hold for all $b < a_0$ and it is this result which is our

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main concern here. Our proof of a pointwise bound with b arbitrarily close to a_0 appears in §3.

Independently of Ahlrichs, A. O'Connor [3], [4] proved that $\exp(a|x|)\Psi \in L^2$ for $a < a_0$. O'Connor's method is very elegant, and his result is much more general than Ahlrichs requiring very minimal hypotheses on the potentials. Our proof in §3 will result by a simple synthesis of our version of Kato's Hölder continuity theorem and O'Connor's methods.

In §4, we give a brief discussion of the extension of our results to the situation where the pair potentials are in \mathbb{R}^n ($n \neq 3$) or where the Hamiltonian must be defined as a sum of quadratic forms [5].

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2. Kato's Hölder continuity theorem. Throughout this section, H_0 represents an operator on $L^2(\mathbb{R}^{3N-3})$ of the form $H_0 = -\sum_{i,j=1}^{3N-3} a_{ij} \partial_i \partial_j$ where a_{ij} is a positive definite matrix. We write $h(k) \equiv \sum a_{ij} k_i k_j$.

DEFINITION. Let $2 \leq \sigma \leq \infty$. We say that V is a potential of type M_σ if $V = W + \sum_{\alpha \in I} Y_\alpha$ where I is a finite index set and

- (1) \hat{W} is in $L^1(\mathbb{R}^{3N-3})$;
- (2) for each $\alpha \in I$, there is a projection P_α onto some \mathbb{R}^3 in \mathbb{R}^{3N-3} so that $Y_\alpha(x) = Z_\alpha(P_\alpha x)$ where Z_α is a function on \mathbb{R}^3 with $\hat{Z}_\alpha \in L^r + L^1$ where $r^{-1} + \sigma^{-1} = 1$.

REMARKS. (1) $\hat{}$ denotes the Fourier transform.

(2) By the Hausdorff-Young inequality, $Z_\alpha \in L^\sigma + L^\infty \subset (L^2 + L^\infty)(\mathbb{R}^3)$ so V is H_0 -bounded with arbitrary small bound (alternately, see Lemma 1 below). Thus $H_0 + V \equiv H$ defines a selfadjoint operator on $D(H_0)$.

(3) Condition M_σ should be compared to Kato's condition in [2], that $W \in L^\infty$, $Z_\alpha \in (L^\sigma)_0$, the L^σ functions of bounded support. Kato's conditions and M_σ are roughly comparable, but for example if $Z_\alpha(x) = \sin(|x|)$, V obeys Kato's conditions but not M_σ ; if

$$Z_\alpha(x) = \sum_{n=1}^{\infty} C_n |x - r_n|^{-1} \quad \text{where } \sum |C_n| < \infty \text{ and } r_n \rightarrow \infty,$$

then V obeys M_σ but not Kato's conditions. In any event, either allows Yukawa or Coulomb pair interactions.

DEFINITION. $C_\theta(\mathbb{R}^n)$ ($0 < \theta < 1$) denotes the uniformly Hölder continuous functions of order θ , i.e. $\Psi \in C_\theta$ if and only if

$$|\Psi(x) - \Psi(y)| \leq M |x - y|^\theta$$

for some M and (almost) all $x, y \in \mathbb{R}^n$. Similarly $\Psi \in C'_\theta(\mathbb{R}^n)$ means Ψ is continuously differentiable and for each $i = 1, \dots, n$, $\partial_i \Psi \in C_\theta$.

THEOREM 1. *Let $H=H_0+V$ where V is of type M_σ . Then:*

- (1) *If $\sigma \geq 2$, any $\Psi \in C^\infty(H) \equiv \bigcap_m D(H^m)$ is in $C_\theta(\mathbb{R}^{3N-3})$ for any $\theta < \min(1, 2-3\sigma^{-1})$.*
- (2) *If $\sigma > 3$, any $\Psi \in C^\infty(H)$ is in $C'_\theta(\mathbb{R}^{2N-3})$ for any $\theta < 1-3\sigma^{-1}$.*

REMARKS. (1) As we shall see, the condition $\Psi \in C^\infty(H)$ can be replaced with $\Psi \in D(H^m)$ for some m with $(m-1)(4-6\sigma^{-1}) > 3N-3$.

(2) If $C^\infty(H)$ is topologized with the norms $\|\Psi\|_m = \|H^m\Psi\|$ and if C_θ (resp. C'_θ) is topologized with the norm

$$\|f\|_\theta = \sup_x |f(x)| + \sup_{x,y} [|x - y|^{-\theta} |f(x) - f(y)|]$$

(resp. $\|f\|'_\theta = \sup_x |f(x)| + \sum_{j=1}^n \|\partial_j f\|_\theta$), then the imbeddings $C^\infty(H) \subset C_\theta$ guaranteed by the theorem are continuous.

(3) Except for a slight difference in the assumptions on V , this is the main theorem (Theorem I) of [2].

(4) The basic perturbation estimate tells us that $(H_0+I)^{-1}V$ is bounded from L^2 to L^2 . Our proof (like Kato's) is based on two ways in which this can be improved. First $(H_0+I)^{-\beta}V$ is bounded for certain $\beta < 1$ and secondly it is bounded on certain L^p spaces.

LEMMA 1. *Let V be of type M_σ and let $\beta > 3/2\sigma$. Suppose that $1 \leq p \leq 2$ and let $\hat{\Psi} \in L^p$. Then $((H_0+I)^{-\beta}V\Psi)^\wedge \in L^p$.*

REMARK. This lemma (and similar statements later) are intended to hold in the sense of a priori estimates

$$\|((H_0 + I)^{-\beta}V\Psi)^\wedge\|_p \leq C \|\hat{\Psi}\|_p$$

for all $\Psi \in \mathcal{S}(\mathbb{R}^{3N-3})$.

PROOF.

$$((H_0 + I)^{-\beta}V\Psi)^\wedge = (2\pi)^{(3N-3)/2}(h(k) + 1)^{-\beta}\hat{V} * \hat{\Psi}.$$

We consider the individual terms $\hat{W} * \hat{\Psi}$ and $\hat{Y}_\alpha * \hat{\Psi}$ in $\hat{V} * \hat{\Psi}$. Since $\hat{W} \in L^1$ and $(h(k) + 1)^{-\beta} \in L^\infty$,

$$\|(h(k) + 1)^{-\beta}\hat{W} * \hat{\Psi}\|_p \leq \|(h(k) + 1)^{-\beta}\|_\infty \|\hat{W}\|_1 \|\hat{\Psi}\|_p$$

by Young's and Hölder's inequalities.

Write k_α for the 3 coordinates in $\text{Ran } P_\alpha$ and k_α^\perp for $3N-6$ orthogonal coordinates. Since $(k_\alpha^2 + 1)^{-\beta} \in L^\sigma(\mathbb{R}^3)$ for each $p \leq \sigma$,

$$\|(k_\alpha^2 + 1)^{-\beta}(\hat{Z}_\alpha * f)(k_\alpha)\|_p \leq C \|f\|_p.$$

Thus for each $p \leq 2$ and each fixed k_α^\perp :

$$\int \left| (k_\alpha^2 + 1)^{-\beta} \int \mathcal{Z}_\alpha(k_\alpha - k'_\alpha) f(k'_\alpha, k_\alpha^\perp) dk'_\alpha \right|^p dk_\alpha \leq C \int |f|(k_\alpha, k_\alpha^\perp)|^p dk_\alpha.$$

Integrating over k_α^\perp , we conclude that $\|(k_\alpha^2+1)^{-\beta} \hat{Y}_\alpha * \hat{\Psi}\|_p \leq C_1 \|\hat{\Psi}\|_p$. Since $(k_\alpha^2+1)^\beta (h(k)+1)^{-\beta} \in L^\infty(\mathbb{R}^{3N-3})$, the lemma follows. \square

LEMMA 2. Let V be of type M_σ and let $\gamma < 1 - 3/2\sigma$. Let $1 \leq p \leq 2$. If $\hat{\Psi}, (H\Psi)^\wedge \in L^p$, then $(1+|k|^2)^\gamma \hat{\Psi} \in L^p$.

PROOF. Since $(H+1)\Psi = (H_0+1)\Psi + V\Psi$, we have $\Psi = (H_0+1)^{-1} \times (H+1)\Psi - (H_0+1)^{-1}V\Psi$. So:

$$(2) \quad (1+|k|^2)^\gamma \hat{\Psi} = (1+|k|^2)^{\gamma-1} [(1+|k|^2)/(1+h(k))((H+1)\Psi)^\wedge - [(1+|k|^2)/(1+h(k))]^\gamma ((H_0+1)^{-\beta}V\Psi)^\wedge$$

where $\beta = 1 - \gamma > 3/2\sigma$. By hypothesis, the first term on the right-hand side of (2) is in L^p and by Lemma 1, the second term is in L^p . \square

For the reader's convenience, we include the following standard result:

LEMMA 3. If $(1+|k|^2)^\gamma \hat{\Psi} \in L^1(\mathbb{R}^n)$ for $\gamma > 0$, then Ψ is C_θ for any θ with $\theta < \min(1, 2\gamma)$. If $\gamma > \frac{1}{2}$, then Ψ is C_θ' for any $\theta < \min(1, 2\gamma - 1)$.

PROOF. For any $y \in \mathbb{R}$, $|e^{iy} - 1| \leq 2$ and $|e^{iy} - 1| = |\int_0^y e^{ix} dx| \leq y$. Therefore, for any $\theta \leq 1$ and all k, x and $y \in \mathbb{R}^n$, $|e^{ik \cdot x} - e^{ik \cdot y}| \leq 2^{(1-\theta)} |k|^\theta |x - y|^\theta$. Thus:

$$|\Psi(x) - \Psi(y)| \leq (2\pi)^{-n/2} 2^{1-\theta} |x - y|^\theta \| |k|^\theta (1+|k|^2)^{-\gamma} \|_\infty \|(1+|k|^2)^\gamma \hat{\Psi}\|_1.$$

This proves the first statement in the lemma. The second has a similar proof using

$$|e^{iy} - 1 - iy| \leq 2|y| \quad \text{and} \quad |e^{iy} - 1 - iy| \leq \frac{1}{2}|y|^2. \quad \square$$

PROOF OF THEOREM 1. Since $(1+|k|^2)^{-\gamma} \in L^q(\mathbb{R}^n)$ for all $q > n/2\gamma$, Lemma 2 implies that if $\hat{\Psi}, (H\Psi)^\wedge \in L^p$, then $\hat{\Psi} \in L^r$ for all $r \geq 1$ obeying $r \geq (p^{-1} + (2\gamma/(3N-3)))^{-1}$. By induction if $m \geq k$ and if $\hat{\Psi}, \dots, (H^m\Psi)^\wedge \in L^2$ then $\hat{\Psi}, \dots, (H^k\Psi)^\wedge \in L^r$ if $r \geq 1$ and $r \geq (\frac{1}{2} + (m-k)(2\gamma/(3N-3)))^{-1}$. Since γ can be chosen arbitrarily close to $1 - 3/2\sigma$, we have that for any integer m with $(2m)(2 - 3/\sigma) > 3N - 3$,

- (i) $\Psi \in D(H^m)$ implies $\hat{\Psi} \in L^1$;
- (ii) $\Psi \in D(H^{m+1})$ implies that $(1+|k|^2)^\gamma \hat{\Psi} \in L^1$ if $\gamma < 1 - 3/2\sigma$.

Lemma 3 completes the proof. \square

3. Pointwise exponential falloff of discrete eigenfunctions. By an N -body quantum Hamiltonian of type M_σ , we will mean an operator \tilde{H} on $L^2(\mathbb{R}^{3N})$ of the form

$$\tilde{H} = -\sum_{i=1}^N (2m_i)^{-1} \Delta_i + \sum_{i < j=1}^N V_{ij}(r_i - r_j).$$

Where a point in \mathbf{R}^{3N} is written (r_i, \dots, r_N) with $r_i \in \mathbf{R}^3$, Δ_i is the Laplacian with respect to r_i and V_{ij} is a function on \mathbf{R}^3 with $\hat{V}_{ij} \in L^q + L^1$ where $q^{-1} + \sigma^{-1} = 1$.

Write $M = \sum_{i=1}^N m_i$ (total mass), $\mathbf{R} = M^{-1} \sum_{i=1}^N m_i r_i$ (center of mass) and

$$x = \left(\sum_{i=1}^N m_i M^{-1} |r_i - \mathbf{R}|^2 \right)^{1/2}$$

(radius of gyration). In a standard way we can choose linear coordinates $(\zeta_1, \dots, \zeta_{N-1}, R)$ so that under the resulting decomposition

$$L^2(\mathbf{R}^{3N}) = L^2(\mathbf{R}^{3N-3}) \otimes L^2(\mathbf{R}^3),$$

$$\tilde{H} = H \otimes 1 + 1 \otimes (2M)^{-1} \Delta.$$

We will call H a *reduced N -body quantum Hamiltonian of type M_σ* . Such a Hamiltonian is always of the form $H_0 + V$ where V is a potential of type M_σ in the sense of §2. By a further linear coordinate change (of Jacobian not necessarily 1), we can suppose that $x^2 = \sum_{i=1}^{N-1} |\zeta_i|^2$ in which case

$$H_0 = (-2M)^{-1} \sum_{i=1}^{N-1} \Delta_{\zeta_i}.$$

THEOREM 2. *Let H be a reduced N -body quantum Hamiltonian of type M_σ . Let $E_c = \inf \sigma_{\text{ess}}(H)$ and suppose that $H\Psi = E\Psi$ with $E < E_c$. Let $a_0 = (2M(E_c - E))^{1/2}$ and let $|x|$ be the radius of gyration. Then*

(1) *For any $a_1 < a_0$, there exists a constant D_{a_1} with*

$$|\Psi(\zeta)| \leq D_{a_1} \exp(-a_1 |x|)$$

for all $\zeta \in \mathbf{R}^{3N-3}$.

(2) *For any $a_1 < a_0$, and $\theta < \min(1, 2 - 3\sigma^{-1})$, there exists a constant D_{θ, a_1} with*

$$|\Psi(\zeta) - \Psi(\zeta')| \leq D_{\theta, a_1} \exp[-a_1 \min(|\zeta|, |\zeta'|)] |\zeta - \zeta'|^\theta$$

for all $\zeta, \zeta' \in \mathbf{R}^{3N-3}$.

(3) *If $\sigma > 3$, for any $a_1 < a_0$, and $\theta < 1 - 3\sigma^{-1}$, there exists D'_{θ, a_1} with*

$$|\text{grad } \Psi(\zeta) - \text{grad } \Psi(\zeta')| \leq D'_{\theta, a_1} \exp[-a_1 \min(|\zeta|, |\zeta'|)] |\zeta - \zeta'|^\theta$$

for all $\zeta, \zeta' \in \mathbf{R}^{3N-3}$.

REMARK. The constants, D_{a_1} , D_{θ, a_1} and D'_{θ, a_1} depend on V only through L^p norms of the \hat{V}_{ij} .

PROOF. Suppose H is in normal form. By a Payley-Wiener argument (see, e.g. O'Connor [3], [4]), we need only prove that $\hat{\Psi}$ has an analytic continuation to the tube $\{k \in \mathbf{C}^{3N-3} \mid |\text{Im } k| < a_0\}$ so that if $\hat{\Psi}_a$ is defined by $\hat{\Psi}_a(k) = \hat{\Psi}(k + ia)$ for any $a \in \mathbf{R}^{3N-3}$ with $|a| < a_0$, then $(1 + k^2)^\nu \hat{\Psi}_a \in L^1$

with L^1 norm bounded as a runs through the set $\{a \mid |a| < a_1\}$ for each $a_1 < a_0$. Here γ is any real less than $1 - 3/2\sigma$.

O'Connor [3], [4] has already proven that such a continuation exists with $\hat{\Psi}_a \in L^2$ uniformly as a runs through sets of the form $\{a \mid |a| < a_1\}$. Moreover $\hat{\Psi}_a$ obeys the equation

$$(3) \quad ((k + ia)^2 - E)\hat{\Psi}_a = (2\pi)^{(3N-3)/2} \hat{V} * \hat{\Psi}_a.$$

By mimicking our argument in §2, the equation (3), the condition that V be of type M_σ and O'Connor's L^2 bounds imply the required L^1 bound on $(1+k^2)^\gamma \hat{\Psi}$. \square

4. Extension to higher dimensions and to operators defined by quadratic forms. In this section, we wish to generalize Theorem 1; a similar generalization of Theorem 2 holds. Since there are few new ideas, we only sketch the arguments.

DEFINITION. Let $\sigma \geq 1$. We say that V is a potential of type $M_\sigma^{(m)}$ on \mathbb{R}^{mN-m} if $V = W + \sum_{\alpha \in I} Y_\alpha$ where I is a finite index set and if

- (1) $W \in L^1(\mathbb{R}^{mN-m})$.
- (2) For each $\alpha \in I$, there is a projection P_α onto an \mathbb{R}^m in \mathbb{R}^{mN-m} and a function Z_α on \mathbb{R}^m with $\hat{Z}_\alpha \in L^r + L^1(r^{-1} + \sigma^{-1} = 1)$ so that $Y_\alpha(x) = Z_\alpha(P_\alpha x)$.

If $\sigma \geq 2$ and $\sigma > m/2$, then $H_0 + V$ can be defined as a selfadjoint operator sum. If $2 > \sigma > m/2$ (in particular, only when $m \leq 3$), we can define $H_0 + V$ as a selfadjoint operator which is the sum of H_0 and V as quadratic forms [5]. We have:

THEOREM 1'. Let $H = H_0 + V$ where V is of type $M_\sigma^{(m)}$ with $\sigma > m/2$ (and $\sigma \geq 1$). Then:

- (1) Any $\Psi \in C^\infty(H)$ is in $C_\theta(\mathbb{R}^{mN-m})$ for any $\theta < \min(1, 2 - m\sigma^{-1})$.
- (2) If $\sigma > m$, any $\Psi \in C^\infty(H)$ is in $C'_\theta(\mathbb{R}^{mN-m})$ for any $\theta < 1 - m\sigma^{-1}$.

SKETCH OF PROOF. Case 1: $\sigma > 2$. Our proof of Theorem 1 goes through with minor modifications; Lemma 1 holds if $\beta > m/2\sigma$ and Lemma 2 if $\gamma < 1 - m/2\sigma$. The condition $\sigma \geq 2$ enters in the proof of Lemma 1, since to apply Young's inequality to $L^p * L^q$ we need $p^{-1} + q^{-1} > 1$.

Case 2: $2 \geq \sigma > m/2$. A simple quadratic form modification. We first note that Lemma 1 holds if $\beta > m/2\sigma$ and if $p \leq \sigma$. Moreover, we have:

LEMMA 1'. Let $\sigma \leq p \leq 2$ and define α by $\alpha^{-1} + \sigma/p = 1$. Let $\beta > m/2\sigma$ and let $\hat{\Psi} \in L^p$. Then the Fourier transform of $(H_0 + 1)^{-(1-\alpha)\beta} V (H_0 + 1)^{-\alpha\beta} \Psi$ is in L^p .

LEMMA 2'. Let p, σ, α, β be as in Lemma 1'. Suppose that $(1+k^2)^{\alpha\beta} \hat{\Psi}, (H\Psi)^\wedge \in L^p$. Let $\gamma < 1 - m/2\sigma$. Then $(1+k^2)^\gamma (1+k^2)^{\alpha\beta} \hat{\Psi} \in L^p$.

The proofs of Lemmas 1' and 2' follow the pattern of Lemmas 1 and 2. If $\Psi \in C^\infty(H)$, then $H^n \Psi \in Q(H)$, the form domain of H for each n . Since $Q(H) = Q(H_0)$, $(1+k^2)^{1/2}(H^n \Psi)^\wedge \in L^2$ for all n . By a finite induction using Lemma 2', $(H^n \Psi)^\wedge \in L^\sigma$. Lemma 1 is now applicable and the proof is completed as in Theorem 1. \square

One can ask if some modified version of Theorem 1' remains true at the borderline value $\sigma = m/2$. If $m \geq 5$, $H_0 + V$ can be defined as an operator sum if V is of type $M_{m/2}^{(m)}$ and if $m = 2, 3, 4$, $H_0 + V$ can be defined as a sum of forms. However, in this borderline case, there may be unbounded functions $\Psi \in C^\infty(H)$.

EXAMPLE. Let $m \geq 3$ and let Ψ be a spherically symmetric function on \mathbf{R}^m so that (i) Ψ is C^∞ and strictly positive on $\mathbf{R}^m \setminus \{0\}$. (ii) In the region $R_1 = \{x \mid |x| \geq 1\}$ Ψ obeys $-\Delta \Psi = -\Psi$ and $\Psi \rightarrow 0$ as $|x| \rightarrow \infty$. (iii) In the region $R_2 = \{x \mid |x| \leq \frac{1}{2}\}$, $\Psi(x) = -\ln|x|$. It is easy to construct such a function. Let $V(x) = -1 + (\Delta \Psi / \Psi)$. Then V has support in $\mathbf{R}^m \setminus R_1$, and in the region R_2 , $V(x) = -1 + C_m r^{-2} (\ln r)^{-1}$. Thus $V \in L^{m/2}$ (and in particular, if $m = 3$, $V \in R$, the Rollnik class [5]) and Ψ is in $C^\infty(H)$ and is unbounded.

REMARK. The above example does not work in case $m = 2$, because $-\Delta(\ln r) = C_2 \delta(x)$; but if we modify Ψ to equal $(-\ln|x|)^\alpha$ with $0 < \alpha < 1$ in R_2 , then $V = -1 + d_\alpha r^{-2} (\ln r)^{-2}$ in R_2 so $V \in L^1(\mathbf{R}^2)$. Thus there is a borderline example in \mathbf{R}^2 .

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