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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

$$|\Psi(\zeta)| \leqq D_\varepsilon \exp[-(1-\varepsilon)a_0|x|]$$

on discrete eigenfunctions of energy E. Here $\varepsilon>0$, $a_0^2=2$ (mass of the system) [dist(E, σ_{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 $\boldsymbol{R}^{3N-3}$ 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 $|x|\to\infty$ 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

$$(1) \qquad |\Psi(x)| \leqq C_b \exp(-b\,|x|)$$

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 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 $L^2(R^{3N-3})$ 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 $h(k)\equiv\sum a_{ij}k_ik_j$.

DEFINITION. Let $2\leqq\sigma\leqq\infty$. 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 $L^1(R^{3N-3})$;

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

REMARKS. (1) ^ denotes the Fourier transform.

(2) By the Hausdorff-Young inequality, $Z_\alpha\in L^\sigma+L^\infty\subset(L^2+L^\infty)(R^3)$ 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

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

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

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

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

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

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

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

(2) *If* $\sigma>3$, *any* $\Psi\in C^\infty(H)$ *is in* $C'_\theta(\boldsymbol{R}^{2N-3})$ *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 $1\leqq p\leqq 2$ and let $\hat{\Psi}\in L^p$. Then $((H_0+I)^{-\beta}V\Psi)\hat{}\in L^p$.*

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

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

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

PROOF.

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

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 $(h(k)+1)^{-\beta}\in L^\infty$,

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

by Young's and Hölder's inequalities.

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

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

Thus for each $p\leqq 2$ and each fixed $k_\alpha^\perp$:

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

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

LEMMA 2. *Let V be of type M_σ and let $\gamma<1-3/2\sigma$. Let $1\leqq p\leqq 2$. If $\hat{\Psi}$, $(H\Psi)\hat{}\in L^p$, 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:

$$(2)\qquad \begin{aligned}(1+|k|^2)^\gamma\hat{\Psi} = {}&(1+|k|^2)^{\gamma-1}[(1+|k|^2)/(1+h(k)]((H+1)\Psi)\hat{}\\ &-[(1+|k|^2)/(1+h(k))]^\gamma((H_0+1)^{-\beta}V\Psi)\hat{}\end{aligned}$$

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. □

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

LEMMA 3. *If $(1+|k|^2)^\gamma\hat{\Psi}\in L^1(\mathbf{R}^n)$ 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 $y\in\mathbf{R}$, $|e^{iy}-1|\leqq 2$ and $|e^{iy}-1|=|\int_0^y e^{ix}\,dx|\leqq y$. Therefore, for any $\theta\leqq 1$ and all k, x and $y\in\mathbf{R}^n$, $|e^{ik\cdot y}-e^{ik\cdot y}|\leqq 2^{(1-\theta)}|k|^\theta|x-y|^\theta$. Thus:

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

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

$$|e^{iy}-1-iy|\leqq 2\,|y| \quad\text{and}\quad |e^{iy}-1-iy|\leqq \tfrac{1}{2}\,|y|^2. \quad □$$

PROOF OF THEOREM 1. Since $(1+|k|^2)^{-\gamma}\in L^q(\mathbf{R}^n)$ for all $q>n/2\gamma$, Lemma 2 implies that if $\hat{\Psi}$, $(H\Psi)\hat{}\in L^p$, then $\hat{\Psi}\in L^r$ for all $r\geqq 1$ obeying $r\geqq(p^{-1}+(2\gamma/(3N-3)))^{-1}$. By induction if $m\geqq k$ and if $\hat{\Psi},\cdots,(H^m\Psi)\hat{}\in L^2$ then $\hat{\Psi},\cdots,(H^k\Psi)\hat{}\in L^r$ if $r\geqq 1$ and $r\geqq(\frac{1}{2}+(m-k)(2\gamma/(3N-3)))^{-1}$. 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. □

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 $L^2(\mathbf{R}^{3N})$ of the form

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

Where a point in $\boldsymbol{R}^{3N}$ is written $(\boldsymbol{r}_i, \cdots, \boldsymbol{r}_N)$ with $\boldsymbol{r}_i \in \boldsymbol{R}^3$, Δ_i is the Laplacian with respect to r_i and V_{ij} is a function on $\boldsymbol{R}^3$ 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), $\mathbf{R}=M^{-1}\sum_{i=1}^N m_i \boldsymbol{r}_i$ (center of mass) and

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

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

$$L^2(\boldsymbol{R}^{3N}) = L^2(\boldsymbol{R}^{3N-3}) \otimes L^2(\boldsymbol{R}^3),$$
$$\tilde{H} = H \otimes 1 + 1 \otimes (2M)^{-1}\Delta.$$

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*

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

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

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

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

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

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

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

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

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 $\{k \in \boldsymbol{C}^{3N-3} \mid |\text{Im}\, k|<a_0\}$ so that if $\hat{\Psi}_a$ is defined by $\hat{\Psi}_a(k)=\hat{\Psi}(k+i\boldsymbol{a})$ for any $\boldsymbol{a} \in \boldsymbol{R}^{3N-3}$ with $|\boldsymbol{a}|<a_0$, then $(1+k^2)^\gamma\hat{\Psi}_a \in L^1$

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

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

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 $(1+k^2)^\gamma \hat{\Psi}$. □

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

(1) $\hat{W} \in L^1(\mathbf{R}^{mN-m})$.

(2) For each $\alpha \in I$, there is a projection P_α onto an $\mathbf{R}^m$ in $\mathbf{R}^{mN-m}$ and a function Z_α on $\mathbf{R}^m$ 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 $\sigma \geqq 2$ 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 $m \leqq 3$), 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 $\sigma \geqq 1$). Then:*

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

(2) If $\sigma > m$, any $\Psi \in C^\infty(H)$ is in $C'_\theta(\mathbf{R}^{mN-m})$ 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 $\sigma \geqq 2$ 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: $2 \geqq \sigma > m/2$. A simple quadratic form modification. We first note that Lemma 1 holds if $\beta > m/2\sigma$ and if $p \leqq \sigma$. Moreover, we have:

LEMMA 1′. *Let $\sigma \leqq p \leqq 2$ 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. □

One can ask if some modified version of Theorem 1′ remains true at the borderline value $\sigma=m/2$. If $m\geqq 5$, 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 $m\geqq 3$ and let Ψ be a spherically symmetric function on $\boldsymbol{R}^m$ so that (i) Ψ is C^∞ and strictly positive on $\boldsymbol{R}^m\backslash\{0\}$. (ii) In the region $R_1=\{x \mid |x|\geqq 1\}$ Ψ obeys $-\Delta\Psi=-\Psi$ and $\Psi\to 0$ as $|x|\to\infty$. (iii) In the region $R_2=\{x \mid |x|\leqq\frac{1}{2}\}$, $\Psi(x)=-\ln|x|$. It is easy to construct such a function. Let $V(x)=-1+(\Delta\Psi/\Psi)$. Then V has support in $\boldsymbol{R}^m\backslash R_1$, 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 $V\in L^1(\boldsymbol{R}^2)$. Thus there is a borderline example in $\boldsymbol{R}^2$.

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