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ABSTRACT. If H is a possibly unbounded selfadjoint operator and A is a closed operator in a Hilbert space, the relation $(U_t^{-1}AU_tf)'=iU_t^{-1}(AH-HA)U_tf$ can be shown to hold under relatively reasonable hypotheses on A and f, where $U_t=e^{iHt}$. This relation can then be used to relate properties of the commutator $AH-HA$ to properties of A and H.

In quantum mechanics, a state f at time $t=0$ evolves at time t_0 into the state $U_{t_0}f$, where $U_t=e^{iHt}$ and H is the quantum mechanical Hamiltonian operator for the system. This means that for the observable A, the expectation of A in the state U_tf is given by (AU_tf, U_tf). Equivalently, we may regard the state as fixed and the observable A as evolving with time. Thus at time t the new observable A_t is $U_t^{-1}AU_t$. To analyze this evolution further, an obvious step is to differentiate with respect to t, which yields the formal relation $A_t'=iU_t^{-1}(AH-HA)U_t$. If $i(AH-HA)$ is positive definite, for example, this means that expectations are increasing.

Thus one is naturally led to study the commutator $AH-HA$. We shall use the group U_t as an essential tool in our study, and the hypotheses of our theorems will explicitly involve U_t. This seems justified physically, since U_t has direct physical significance.

A quite different method of relating A, H and $AH-HA$ is given in the interesting book by Putnam [3].

In what follows, we let $U_t=e^{iHt}$, and H be a selfadjoint operator in a Hilbert space h. A will be a closed operator in h. Take domain H^∞ to mean the intersection of the domains of all H^n, where n ranges over the positive integers. Take H^0 to be the identity operator.

We first state and prove conditions under which the relationship $(U_t^{-1}AU_t)'=iU_t^{-1}(AH-HA)U_t$ holds.

THEOREM 1. *Let n be a nonnegative integer, and let $m>n$ be a positive integer or ∞. Suppose that domain A contains domain H^n, and that A takes*

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domain H^m into domain H. Then, for any f in domain H^m, $(U_t^{-1}AU_tf)'$ exists in the strong sense and is equal to $i[U_t^{-1}(AH-HA)U_t]f$.

REMARK. If AH and HA were both defined on domain H^i, for some nonnegative integer i, the hypotheses of Theorem 1 would hold, taking $n=i$, and $m=i+1$.

PROOF. We prove the theorem by taking difference quotients, after first observing that U_t takes domain H^i onto itself, for any i which is either a nonnegative integer or ∞.

Now

$$U_{t+\Delta t}^{-1}AU_{t+\Delta t}f - U_t^{-1}AU_tf = U_t^{-1}[U_{\Delta t}^{-1}AU_{\Delta t} - A]U_tf.$$

Calling $U_tf=g$, we note that g is in domain H^m. But

$$\begin{aligned}(1/\Delta t)&[U_{\Delta t}^{-1}AU_{\Delta t} - A]g\\ &= (1/\Delta t)(U_{-\Delta t} - I)Ag + (U_{-\Delta t}A(U_{\Delta t} - I)g)(1/\Delta t).\end{aligned}$$

As Δt approaches zero, the first term goes to $-iHAg$, since Ag is in domain H by hypothesis. The second term is a little harder to analyze.

First, we note that A defines a closed, and therefore continuous linear transformation of B into h, where B is the Banach space created by giving domain H^n the graph norm associated with H^n.

However $(U_{\Delta t}-I)g/\Delta t$ approaches iHg in B as Δt approaches zero, since g is in domain H^{n+1}. Thus $A(U_{\Delta t}-I)g/\Delta t$ converges to $iAHg$ in h. But, finally, from strong continuity of U_t and the fact that $\|U_t\|=1$ for all t, it follows that $U_{-\Delta t}A(U_{\Delta t}-I)(g/\Delta t)$ approaches $iAHg$ as Δt approaches zero.

Collecting what we have proved, we see that $(1/\Delta t)[U_{-\Delta t}AU_{\Delta t}-A]g$ approaches $i(AH-HA)g$ as Δt approaches zero. From continuity of U_t it follows that $(1/\Delta t)U_{-t}(U_{-\Delta t}AU_{\Delta t}-A)U_tf$ approaches $iU_{-t}(AH-HA)U_tf$ in h as Δt approaches zero. This completes the proof of Theorem 1.

COROLLARY 1. *Under the hypotheses of Theorem 1, it cannot happen that $(i(AH-HA)U_tf, U_tf)>C\|U_tf\|^2$ for any $C>0$, and neither can it happen that $(i(AH-HA)U_tf, U_tf)<-C\|U_tf\|^2$ for all t in any infinite interval.*

PROOF. By the closed graph theorem, and the fact that in the graph norm generated by H on domain H, the norm of U_tf is the same as that of f, it follows that $\|AU_tf\|$ remains bounded. Therefore so does (AU_tf, U_tf). By Theorem 1, the proof is completed.

DEFINITION. An operator A is said to be local with respect to U_tf if U_tf is contained in domain A for all t, and AU_tf approaches zero as t approaches $\pm\infty$.

It might at first appear that it is hard to show that an operator A is local with respect to $U_t f$. This is not the case, however, for many types of selfadjoint operators H which are important in applications. A few remarks on this problem seem in order.

First, if H is a selfadjoint operator in h, and f is an element of h, then recall that f is said to be absolutely continuous with respect to H if the real valued measure $m_f(S)=\|P(S)f\|^2$ is absolutely continuous with respect to Lebesgue measure on R. Here S is any borel set in R, and $P(S)$ is the projection associated with S by the spectral measure associated with H. The set of all such f forms a reducing subspace of H, and the restriction of H to this subspace forms a selfadjoint operator H_a. U_t takes this subspace into itself. If $H_a=H$, H is said to be absolutely continuous.

Now, if f is absolutely continuous with respect to H, H is a selfadjoint ordinary differential operator and $h=L_2(R)$, it follows by an argument in Lax and Phillips [**2**, p. 147], that $\|C_\Delta U_t f\|$ approaches 0 as t approaches $\pm\infty$, where C_Δ is the characteristic function of any compact interval Δ. Here H must be assumed to have order one or greater. Thus if A is a bounded operator, and A is the limit in operator norm of a sequence of operators A_n defined by $A_n f=AC_{\Delta_n}f$ for a sequence of compact intervals Δ_n, it follows that A is local with respect to $U_t f$, provided $U_t=e^{iHt}$, H is a selfadjoint ordinary differential operator, and f is absolutely continuous with respect to H. An example of such an A is multiplication by a C_0 function.

It may be shown (see Kato [**1**]) that many ordinary differential operators have nontrivial absolutely continuous parts, and that therefore such vectors f may be found. Further, similar considerations can be made to apply to the case where A is an ordinary differential operator with C_0 coefficients, provided H is a selfadjoint ordinary differential operator in $L_2(R)$ with bounded coefficients and nontrivial absolutely continuous part and A is of order less than or equal to that of H.

Another way of showing locality, which also applies to differential operators is contained in the following theorem.

THEOREM 2. *Let H be absolutely continuous. Let A be H-compact. Then A is local with respect to $U_t f$ for all f in domain H.*

REMARK. Recall that A is said to be H-compact if domain A contains domain H, and A is a compact operator from domain H into h, where domain H is equipped with the graph norm from H.

PROOF. Since H is absolutely continuous, then by the Riemann-Lebesgue lemma $(U_t f, g)$, which equals $(\int_{-\infty}^{\infty} e^{i\lambda t}\, dP_\lambda f, g)$, approaches 0 when t approaches $\pm\infty$ for all f and g in h. Now suppose A is not local with respect to some f in domain H. Then there is a sequence t_n approaching, say, $+\infty$ such that $\|AU_{t_n}f\|>C$ for some $C>0$. Since A is H-compact, it follows that, for some subsequence $t_{n(j)}$, $AU_{t_{n(j)}}f$ approaches g, with $\|g\|\geqq C$.

Let $U_{t_{n(j)}}f=f_j$. Let $\|Af_j\|\leqq M$. Select g_1 in domain A^* such that $\|g_1-g\|\leqq C^2/2M$. Then $|(Af_j,g_1)-(Af_j,g)|\leqq M\,\|g_1-g\|\leqq C^2/2$. Therefore, when j is large enough, $|(Af_j,g_1)|\geqq C^2/4$. Therefore $|(f_j,A^*g_1)|\geqq C^2/4$, which contradicts the fact f_j converges weakly to 0. This completes the proof.

We now use the hypothesis of locality with respect to U_tf.

THEOREM 3. *Suppose that AH^2, HAH and H^2A are all defined on domain H^{n-1} for some positive integer $n\geqq 3$. Suppose A is local with respect to U_tf, where f is in domain H^n, and suppose there is a dense subspace S of h on which A^*H^2, HA^*H and H^2A^* are defined. Then $AH-HA$ is local with respect to U_tf.*

REMARK. If A is symmetric, the last hypothesis is obviously redundant. Also if A and H are ordinary differential operators, C_0^∞ will usually be such a subspace S.

PROOF. $(U_t^{-1}AU_tf)''=U_t^{-1}(AH^2-2HAH+H^2A)U_tf$ as may be seen using Theorem 1. It is of course necessary to show that the operator $AH-HA$, when restricted to domain H^{n-1}, has a closed extension. However, an operator has a closed extension if and only if its adjoint is densely defined, so our last hypothesis takes care of this possibility.

Now if T is the operator $AH^2-2HAH+H^2A$, restricted to domain H^n, then T has a closed extension. Therefore, giving domain H^n the graph norm from H^n, and letting $\hat{T}$ denote the operator induced by T from this Banach space into H, we see that $\hat{T}$ is continuous by the closed graph theorem.

But since $H^nU_tf=U_tH^nf$, it follows that all U_tf have the same norm as f in the graph norm on domain H^n. Therefore the set of all U_tf is a bounded set in the Banach space domain H^n, so that the set of TU_tf is a bounded set in h. Therefore the set of all $(U_t^{-1}AU_tf)''$ is a bounded set in h, as t ranges over the whole real line.

Let f_t be $U_t^{-1}AU_tf$. We need to show that f_t' approaches zero in norm, as t approaches $\pm\infty$, in order to prove the theorem. Let $g(t)=(f_t,f_t)$. Then $g'(t)=(f_t',f_t)+(f_t,f_t')$. Also, $g''(t)=(f_t'',f_t)+2(f_t',f_t')+(f_t,f_t'')$. Since f_t'' is bounded, and f_t goes to zero as t approaches $\pm\infty$, it follows that (f_t'',f_t) also approaches zero.

To show that (f_t',f_t') approaches 0, we first observe that

$$f_t' = iU_t^{-1}(AH - HA)U_tf,$$

which, once again, by the closed graph theorem, remains bounded as t approaches $\pm\infty$. Thus $(f'_t, f'_t)'$, which equals $(f'_t, f''_t)+(f'_t, f''_t)$, is a bounded real valued function of t. If there were a sequence t_n approaching, say, $+\infty$ such that $(f'_{t_n}, f'_{t_n})>\varepsilon$, then there would have to be a δ such that (f'_t, f'_t) remained $\geqq \varepsilon/2$ on $[t_n-\delta, t_n+\delta]$ for all n, by the mean value theorem. Thus there would be an N such that g'' would be greater than $\varepsilon/4$ on the interval $[t_n-\delta, t_n+\delta]$ for all $n \geqq N$. However, since f_t approaches zero and f'_t remains bounded as t approaches infinity, it is clear that $g'(t)$ must approach 0. This contradicts the fact we just discovered about g''. The theorem is proved.

COROLLARY 2. *Under the hypotheses of Theorem* 3, *it cannot happen that $AH-HA$ has a bounded inverse when restricted to the linear span of the $U_t f$.*

COROLLARY 3. *Let f be as in Theorem* 3, *and suppose f is perpendicular to the eigenvectors of H. Let T be the operator formed by restricting $AH-HA$ to the linear span of the $U_t f$, and T_1 be the closure of the graph of T in the product space $h \times h$. Then T_1 cannot be a linear operator with closed range and finite dimensional null space.*

PROOF. There is a sequence t_n approaching infinity such that $U_{t_n} f$ approaches 0 weakly in h. (See Lax and Phillips [**2**, p. 145].) But $(AH-HA)U_{t_n} f$ approaches zero by Theorem 3.

Let S be the closed linear span of the $U_t f$. If T_1 is a closed operator defined on a dense subspace of S, and K is its null space, and T_1 has closed range, then by dividing out K and using the closed graph theorem we see that the distance from $U_{t_n} f$ to K approaches zero. From this fact, and the fact that K is finite dimensional, it follows that a subsequence of $U_{t_n} f$ converges to a point g of K, with $\|g\|=\|f\|$. This contradicts the weak convergence of $U_{t_n} f$ to zero.

COROLLARY 4. *Let H be absolutely continuous, and A be H-compact and symmetric. Further, suppose that for some positive integer n, AH^2, HAH and H^2A are defined on domain H^n. Then the restriction of $AH-HA$ to domain H^n can have no extension to a closed operator in h with closed range and finite dimensional null space.*

PROOF. Combine Theorem 2 and Corollary 3.

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