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Let A and H be self-adjoint operators on a Hilbert space. Conditions for the differentiability with respect to t of $\langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$ are given, and under these conditions it is shown that the derivative is $\langle i[HA-AH]e^{-itH}\varphi, e^{-itH}\varphi\rangle$. These results are then used to prove Ehrenfest's theorem and to provide results on the behavior of the mean of position as a function of time.

Finally, Stone's theorem on unitary groups is formulated and proved for real Hilbert spaces.

Time Derivatives of Observables and Applications

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TIME DERIVATIVES OF OBSERVABLES AND APPLICATIONS

INTRODUCTION

The Born Interpretation

Let φ be a normalized state function defining the state of a quantum mechanical system. For a long time in the development of quantum mechanics it was not clear how to interpret φ physically. In the 1920's Max Born proposed that $|\varphi|^2$ should be regarded as the probability distribution of the position of the particle in state φ. Thus the probability that the particle is in region R is $\int_R |\varphi|^2 dx$.

Suppose that $H = H_0 + V$ is the Hamiltonian of a particle in a potential field V, then in the Schrodinger picture the fundamental dynamical law of quantum mechanics is that if $\psi(x,t)$ is the state at time t, then $\frac{\partial\psi(x,t)}{\partial t} = iH\psi(x,t)$. That is, $\psi(x,t)$ satisfies the Schrodinger wave equation. Well known considerations connected with Stone's theorem show that the solution in $L^2(R^n)$ is $\psi(x,t) = e^{itH}\varphi$ where φ may be thought of as the initial state at $t = 0$. Thus, $e^{itH}\varphi$ is the state at any time t.

For each t, e^{itH} is unitary, and so if $\|\varphi\| = 1$ then $\|e^{itH}\varphi\|^2 = \langle e^{itH}\varphi, e^{itH}\varphi\rangle = 1$. The Born interpretation now says that some self-adjoint operators can be interpreted as observable quantities. For such an operator A the quantity $\langle Ae^{itH}\varphi, e^{itH}\varphi\rangle$ is the expected value of A when the system is in the state $e^{itH}\varphi$. Indeed, if A is multiplication by x_j, which has a natural interpretation as the j-coordinate of position $(x = (x_1, \ldots, x_n) \in R^n)$, then $\langle x_j e^{itH}\varphi, e^{itH}\varphi\rangle = \int_{R^n} x_j |e^{itH}\varphi|^2 dx$, which is exactly the expected value of the classical position function $x \to x_j$ when $|e^{itH}\varphi|^2$ is viewed as the probability distribution of position at time t.

If we set $\overline{A}(\varphi)(t) = \langle Ae^{itH}\varphi, e^{itH}\varphi\rangle$ then $\overline{A}(\varphi)$ is a real valued function of t. We may therefore ask a very general question: What is the behavior of $\overline{A}(\varphi)(t)$? This paper provides some answers to this general question.

Ehrenfest's Theorem

Consider a particle of mass 1. In classical mechanics $\frac{dx}{dt}$ is the momentum and $\frac{d^2x}{dt^2}$ is the force if $x(t)$ is the position of the particle.

In the quantum mechanics the expected value of momentum in the jth coordinate direction is given by $\langle i \frac{\partial}{\partial x_j} e^{itH}\varphi, e^{itH}\varphi\rangle$. The question arises whether the derivative of the mean of x_j, $(\overline{x}_j'(\varphi)(t))$, is the expected value of momentum. Moreover, is the second derivative of the mean of x_j, $(\overline{x}_j''(\varphi)(t))$, equal to the mean or expected value of the force which is given by $\langle \frac{\partial V}{\partial x_j} e^{itH}\varphi, e^{itH}\varphi\rangle$? Paul

Ehrenfest [9, 455] asserted that the answer is yes! Note that in bibliographic citations the first number locates the reference in the bibliography and the second is the page number. Ehrenfest's justification of his assertion was not rigorous, nor could it be, for he gave no hypotheses. Here we shall give sufficient conditions under which Ehrenfest's Theorem is true.

This will involve us in the question of the differentiability of means to which the bulk of Chapter I is devoted. It is in Chapter II that Ehrenfest's Theorem is taken up.

Bound and Unbound States

The theory of self-adjoint operators on a Hilbert space recognizes both eigenstates and absolutely continuous states. We can ask what the behavior of $\overline{x}_j(\varphi)(t)$ is when φ is an eigenstate or an absolutely continuous state. For an eigenstate, is $\overline{x}_j(\varphi)(t)$ bounded? For an absolutely continuous state, does $\overline{x}_j(\varphi)(t)$ converge to $\pm\infty$ as t converges to $\pm\infty$? We address ourselves to these questions in Chapter II.

In Chapter III we shall give some results on the differentiability of the function $\overline{A}(\varphi)(t)$ where A is assumed bounded. Under this assumption we no longer require A to be self-adjoint.

Stone's Theorem for Real Hilbert Spaces

Let $U(t)$ be a strongly continuous group of unitary operators on a complex Hilbert space. Then Stone's theorem says that $U(t) = e^{itH}$, for some unique self-adjoint operator H, and $U'(t) = iHe^{itH}$. In Chapter IV we shall formulate and prove Stone's theorem for real Hilbert spaces.

To some extent Chapter IV is independent of the preceding chapters. On the other hand, it is quite reasonable to ask about the differentiability of means on real Hilbert spaces. But then a Stone's theorem in the real case becomes indispensable, and so the material of Chapter IV is not as independent of the main theme of this paper as it might at first appear.

I. TIME DERIVATIVES OF UNBOUNDED OBSERVABLES

Let A and H be self-adjoint operators on a Hilbert space $\mathcal{H}$. Consider the expression $\bar{A}(\varphi)(t) = \langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$ defined for $t \in R$. In this chapter we shall provide conditions on A, H and φ such that $\frac{d\bar{A}(\varphi)(t)}{dt} = \bar{A}'(\varphi)(t)$ exists and is equal to $\langle i[HA-AH]e^{-itH}\varphi, e^{-itH}\varphi\rangle$. In particular we shall study the cases where $\mathcal{H} = L^2(R^n)$ and A is a polynomial in $x = (x_1, \ldots, x_n)$, or A is a polynomial in $\frac{\partial}{\partial x} = (\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n})$. In these two cases we shall assume that $H = H_0 + V$ where H_0 is the self-adjoint realization of the Laplacian $-\Delta = -\sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ and V is a suitable potential.

We shall begin by considering any self-adjoint operators A and H on a Hilbert space $\mathcal{H}$. The first theorem gives a general criterion for the differentiability of $\bar{A}(\varphi)(t)$. If A is any operator we shall use $D(A)$ to denote the domain of A. We shall assume all operators are densely defined, but not not necessarily bounded unless it is so stated.

Theorem 1.1. Let A be a symmetric operator and H a self-adjoint operator on a Hilbert space $\mathcal{H}$. Suppose $\varphi \in \mathcal{H}$, $e^{-it_0H}\varphi \in D(HA-AH)$, $e^{-itH}\varphi \in D(A)$, and $\|Ae^{-itH}\varphi\|$ is bounded for all t in a neighborhood of t_0, and $\bar{A}(\varphi)(t) = \langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$.

Then

$$\bar{A}'(\varphi)(t_0) = \langle i[HA-AH]e^{-it_0H}\varphi, e^{-it_0H}\varphi\rangle .$$

<u>Proof</u>. Without loss of generality set $t_0 = 0$, for otherwise we can replace φ by $e^{-it_0H}\varphi$ in the following argument.

$$\begin{aligned}
\bar{A}'(\varphi)(0) &= \lim_{t\to 0} \frac{\langle e^{itH}Ae^{-itH}\varphi, \varphi\rangle - \langle A\varphi, \varphi\rangle}{t} \\
&= \lim_{t\to 0} \left\langle \frac{e^{itH}Ae^{-itH}\varphi - e^{itH}e^{-itH}A\varphi}{t}, \varphi\right\rangle \\
&= \lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - e^{-itH}A\varphi}{t}, e^{-itH}\varphi\right\rangle \\
&= \lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - A\varphi - [e^{-itH}A\varphi - A\varphi]}{t}, e^{-itH}\varphi\right\rangle \\
&= \lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - A\varphi}{t}, e^{-itH}\varphi\right\rangle - \lim_{t\to 0} \left\langle \frac{e^{-itH}A\varphi - A\varphi}{t}, e^{-itH}\varphi\right\rangle \\
&= \lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - A\varphi}{t}, e^{-itH}\varphi\right\rangle + \langle iHA\varphi, \varphi\rangle .
\end{aligned}$$

We next show that

$$\lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - A\varphi}{t}, e^{-itH}\varphi\right\rangle = -\langle iAH\varphi, \varphi\rangle .$$

We have

$$\left| < \frac{Ae^{-itH}\varphi - A\varphi}{t}, e^{-itH}\varphi> - <-iAH\varphi, \varphi> \right|$$

$$= \left| < \frac{e^{-itH}\varphi - \varphi}{t}, Ae^{-itH}\varphi> - <-iH\varphi, Ae^{-itH}\varphi> + <-iH\varphi, Ae^{-itH}\varphi> - <-iH\varphi, A\varphi> \right|$$

since A is symmetric, $H\varphi \in D(A)$, and by adding and subtracting $<-iH\varphi, Ae^{-itH}\varphi>$. Thus,

$$\left| < \frac{Ae^{-itH}\varphi - A\varphi}{t}, e^{-itH}\varphi> - <-iAH\varphi, \varphi> \right|$$

$$\leq \left\| \frac{e^{-itH}\varphi - \varphi}{t} + iH\varphi \right\| \left\| Ae^{-itH}\varphi \right\| + \left\| AH\varphi \right\| \left\| e^{-itH}\varphi - \varphi \right\| .$$

But the right side of this inequality tends to zero as t converges to zero since $\|Ae^{-itH}\varphi\|$ is bounded in a neighborhood of zero.

q.e.d.

<u>Corollary 1.2.</u> If A and H are bounded self-adjoint operators, then $\bar{A}'(\varphi)(t)$ exists for all t, and

$\bar{A}'(\varphi)(t) = <i[HA-AH]e^{-itH}\varphi, e^{-itH}\varphi>$.

Thus, we observe that to establish the differentiability of $\bar{A}(\varphi)(t)$ we must establish the following three things:

1) $e^{-itH}\varphi \in D(A)$ for all t in a neighborhood of t_0,

2) $\|Ae^{-itH}\varphi\|$ is bounded for t in a neighborhood of t_0,

and 3) $e^{-it_0 H}\varphi \in D(HA-AH)$.

To this end we shall have need of the following general concepts and lemmas.

Definition 1.3. Let X be a Banach space and $B : [a, b] \rightarrow X$ be a function on the interval $[a, b]$ with values in X. Then we define

$$\int_a^b B(t)dt = \lim_{\|\Delta t_i\| \to 0} \sum_{i=1}^{n} B(t_i^*)\Delta t_i$$

if the limit exists in norm. This is the usual Riemann integral of a function with values in a Banach space. This integral exists if B is continuous.

Lemma 1.4. Let A be a closed operator on X, and suppose that $\int_a^b B(t)dt$ and $\int_a^b AB(t)dt$ exist. Then $\int_a^b B(t)dt \in D(A)$, and $A\int_a^b B(t)dt = \int_a^b AB(t)dt$.

Proof.

$$A \sum_{n=1}^{n} B(t_i^*)\Delta t_i = \sum_{n=1}^{n} AB(t_i^*)\Delta t_i \ .$$

Now

$$\sum_{n=1}^{n} B(t_i^*)\Delta t_i \rightarrow \int_a^b B(t)dt,$$

and

$$A \sum_{i=1}^{n} B(t_i^*)\Delta t_i = \sum_{i=1}^{n} AB(t_i^*)\Delta t_i \to \int_a^b AB(t)dt \ .$$

But A is closed hence $\int_a^b B(t)dt \in D(A)$, and

$$A\int_a^b B(t)dt = \int_a^b AB(t)dt \ . \qquad \text{q.e.d.}$$

<u>Corollary 1.5.</u> Let A be a closed operator on X, and suppose that the improper integrals $\int_a^\infty B(t)dt$ and $\int_a^\infty AB(t)dt$ exist. Then

$$\int_a^\infty B(t)dt \in D(A), \quad \text{and} \quad A\int_a^\infty B(t)dt = \int_a^\infty AB(t)dt \ .$$

<u>Proof.</u> We have

$$\int_a^\infty B(t)dt = \lim_{b\to\infty} \int_a^b B(t)dt$$

and

$$\int_a^\infty AB(t)dt = \lim_{b\to\infty} \int_a^b AB(t)dt.$$

But,

$$A\int_a^b B(t)dt = \int_a^b AB(t)dt$$

by Lemma 1.4. Thus,

$$\lim_{b \to \infty} A \int_a^b B(t)dt = \int_a^\infty AB(t)dt.$$

Again, A is closed, so

$$\int_a^\infty B(t)dt \in D(A), \quad \text{and} \quad A\int_a^\infty B(t)dt = \int_a^\infty AB(t)dt .$$

q.e.d.

In the sequel we shall often be concerned with integrals over paths in the complex plane of the following type.

Definition 1.6. Let Γ_c be the path defined by $z_1(t) = c + it$ and $z_2(t) = -c + it$ where $t \in (-\infty, \infty)$.

If T is an operator and λ a complex number we shall write $R(\lambda, T) = (\lambda - T)^{-1}$ for the resolvent of T.

We say $f(\lambda)$ is of order $g(\lambda)$ at $\lambda \to \infty$ provided that $\frac{f(\lambda)}{g(\lambda)}$ is bounded for large values of λ.

Lemma 1.7. Let $T(t)$ be a strongly continuous group of unitary operators on the Hilbert space $\mathcal{H}$, and let T be the infinitesimal generator. Let c be a positive real number, and α a complex number with $0 < c < |R(\alpha)|$, $R(\alpha)$ the real part of α. Then, for $\varphi \in D(T^n)$, with n an integer, $n \geq 2$,

$$T(t)\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, T)(\alpha I-T)^n\varphi}{(\alpha-\lambda)^n}\, d\lambda\,.$$

Proof. First we note that $R(\lambda, T) = \int_0^\infty e^{-\lambda t}T(t)dt$, (see [1, 622]), for $\lambda \in \rho(T)$. Moreover, $\|R(\lambda, T)\| \le K\int_0^\infty e^{((c/4)-R(\lambda))t}dt$ for $R(\lambda) > \frac{c}{4}$, so $\|R(\lambda, T)\|$ is uniformly bounded in the half-plane $R(\lambda) > \frac{c}{2}$. Similarly $\|R(\lambda, T)\|$ is uniformly bounded in the half-plane $R(\lambda) < \frac{-c}{2}$. Thus, the integrand is of order $|\lambda|^{-n}$ as $|\lambda| \to \infty$ on Γ_c, and so the integral

$$\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, t)(\alpha I-T)^n\varphi}{(\alpha-\lambda)^n}\, d\lambda$$

is well-defined.

Let $\varphi \in D(T^n)$ and let $B(t)\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, T)(\alpha I-T)^n\varphi}{(\alpha-\lambda)^n}\, d\lambda$.

Now choose μ so that $R(\mu) > c$, and assume $t \ge 0$, then

$$\int_0^\infty e^{-\mu t}B(t)\varphi dt = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, T)(\alpha I-T)^n\varphi}{(\alpha-\lambda)^n}\int_0^\infty e^{(\lambda-\mu)t}dt\, d\lambda$$

$$= \frac{1}{2\pi i}\int_{\Gamma_c} \frac{R(\lambda, T)(\alpha I-T)^n\varphi}{(\mu-\lambda)(\alpha-\lambda)^n}\, d\lambda\,.$$

Because of the order of the integrand this last integral can be replaced by integrals over two small negatively oriented circles about

α and μ. These integrals can then be evaluated by the residues at α and μ.

The Residue at μ: Immediately we see that the residue at μ is

$$\frac{-R(\mu, T)(\alpha I-T)^n \varphi}{(\alpha-\mu)^n}.$$

The Residue at α: Consider

$$f(\lambda) = \frac{R(\lambda, T)}{(\mu-\lambda)(\alpha-\lambda)^n} = \frac{(-1)^{n+1}}{(\lambda-\alpha)^n} \frac{R(\lambda, T)}{(\lambda-\mu)}.$$

We must compute the $(n-1)$-th derivative of $\frac{R(\lambda, T)}{(\lambda-\mu)} = (\lambda-\mu)^{-1} R(\lambda, T)$.

$$\frac{d^{n-1}}{d\lambda^{n-1}} (\lambda-\mu) R(\lambda, T) = \sum_{m=0}^{n-1} \binom{n-1}{m} D^{n-1-m} (\lambda-\mu)^{-1} D^m R(\lambda, T)$$

$$= \sum_{m=0}^{n-1} \binom{n-1}{m} (-1)^{(n-1-m)} \frac{(n-1-m)!}{(\lambda-\mu)^{n-m}} D^m R(\lambda, T),$$

where $D = \frac{d}{d\lambda}$. But $D^m R(\lambda, T) = (-1)^m m! [R(\lambda, T)]^{m+1}$, so

$$\frac{d^{n-1}}{d\lambda^{n-1}} (\lambda-\mu)^{-1} R(\lambda, T) = \sum_{m=0}^{\infty} (-1)^{n-1} (n-1)! \frac{[R(\lambda, T)]^{m+1}}{(\lambda-\mu)^{n-m}}.$$

The residue at α is

$$\sum_{m=0}^{\infty} \frac{(\alpha I-T)^{n-1-m}\varphi}{(\alpha-\mu)^{n-m}} = \frac{\varphi}{(\alpha-\mu)} + \frac{(\alpha I-T)\varphi}{(\alpha-\mu)^2} + \dots + \frac{(\alpha I-T)^{n-1}\varphi}{(\alpha-\mu)^n} .$$

But we have the identity $R(\mu, T)\varphi = \frac{-\varphi}{(\alpha-\mu)} + \frac{(\alpha I-T)R(\mu,T)\varphi}{(\alpha-\mu)}$, so we have in general:

$$\frac{(\alpha I-T)^{k-1}\varphi}{(\alpha-\mu)^k} = -\frac{R(\mu,T)(\alpha I-T)^{k-1}\varphi}{(\alpha-\mu)^{k-1}} + \frac{(\alpha I-T)R(\mu,T)(\alpha I-T)^{k-1}\varphi}{(\alpha-\mu)^k} .$$

Making substitutions and telescoping we get

$$\begin{aligned}\int_0^{\infty} e^{-\mu t}B(t)\varphi dt &= \frac{R(\mu,T)(\alpha I-T)^n\varphi}{(\alpha-\mu)^n} + R(\mu,T)\varphi - \frac{R(\mu,T)(\alpha I-T)^n\varphi}{(\alpha-\mu)^n} \\ &= R(\mu,T)\varphi \\ &= \int_0^{\infty} e^{-\mu t}T(t)\varphi dt .\end{aligned}$$

Now apply linear functionals to both sides to see that $B(t)\varphi = T(t)\varphi$ for all $t \geq 0$ and all $\varphi \in D(T^n)$.

Now $T(-t)$ is a unitary group with generator $-T$. So we have

$$T(-t)\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, -T)(\alpha I+T)^n\varphi}{(\alpha-\lambda)^n} d\lambda$$

for $t \geq 0$. Substituting $-\lambda$ for λ and recalling that

$R(-\lambda, -T) = -R(\lambda, T)$ we see that

$$T(-t)\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{-\lambda t}R(\lambda, T)(\alpha I+T)^n\varphi}{(\alpha-\lambda)^n}\, d\lambda \; .$$

If we put $-\alpha$ for α and $-t$ for t, we get

$$T(t)\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, T)(\alpha I-T)^n\varphi}{(\alpha-\lambda)^n}\, d\lambda \; , \quad \text{for } t \leq 0.$$

Thus, $B(t)\varphi = T(t)\varphi$ for all t. q.e.d.

Lemma 1.8. Let A be a closed operator and H a self-adjoint operator on a Hilbert space $\mathcal{H}$. Let $\varphi \in \mathcal{H}$, and suppose that for an integer $n \geq 2$ and all $\lambda \in \Gamma_c$, $R(\lambda, iH)(\alpha I-iH)^n\varphi \in D(A)$, and $\|AR(\lambda, iH)(\alpha I-iH)^n\varphi\|$ is of order $|\lambda|^{n-(1+\epsilon)}$ as $|\lambda| \to \infty$ on Γ_c for some $\epsilon > 0$, and $AR(\lambda, iH)(\alpha I-iH)^n\varphi$ is continuous in λ on Γ_c. Then for each real t, $e^{itH}\varphi \in D(A)$, and $\|Ae^{itH}\varphi\|$ is bounded on any finite interval as a function of t. Here α is as in Lemma 1.7.

Proof. Note that iH is the infinitesimal generator of the unitary group e^{itH}. From Lemma 1.7 we have

$$e^{itH}\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}R(\lambda, iH)(\alpha I-iH)^n\varphi}{(\alpha-\lambda)^n}\, d\lambda \; .$$

But $\dfrac{e^{\lambda t}AR(h,iH)(\alpha I-iH)^n\varphi}{(\alpha-\lambda)^n}$ is continuous on Γ_c, and its norm is of order $|\lambda|^{-(1+\epsilon)}$ as $|\lambda| \to \infty$ on Γ_c. Thus,

$$\frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}AR(\lambda,iH)(\alpha I-iH)^n\varphi}{(\alpha-\lambda)^n}\,d\lambda$$

exists. Consequently by Corollary 1.5 $e^{itH}\varphi \in D(A)$, and

$$Ae^{itH}\varphi = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}AR(\lambda,iH)(\alpha I-iH)^n\varphi}{(\alpha-\lambda)^n}\,d\lambda \; .$$

But then

$$\|Ae^{itH}\varphi\| \leq \frac{1}{2\pi}\int_{\Gamma_c} |e^{\lambda t}|\,\|AR(\lambda,iH)(\alpha I-iH)^n\varphi\|\,|d\lambda| ,$$

and since $e^{\lambda t} = e^{(\pm c+ib)t}$, where $b \in (-\infty,\infty)$, we have $\|Ae^{itH}\varphi\|$ bounded on any finite interval of the real line. q.e.d.

<u>Remark 1.9.</u> Let V be a closed operator and H self-adjoint. Suppose $D(H) \subset D(V)$. Then $VR(\lambda,iH)$ is a bounded operator, since it is closed and everywhere defined.

<u>Lemma 1.10.</u> Let H_0 and H be self-adjoint operators and V a symmetric operator with $D(H_0) \subset D(V)$. Moreover, let $H = H_0 + V$. Let $\lambda \in \rho(iH_0) \cap \rho(iH)$, the intersection of the resolvent sets of iH_0 and iH, then $R(\lambda,iH) - R(\lambda,iH_0) = R(\lambda,iH_0)iVR(\lambda,iH)$.

Proof. For $\varphi \in D(H_0) = D(H)$ we have $(\lambda - iH_0)\varphi - (\lambda - iH)\varphi = iV\varphi$. But $\varphi = (\lambda - iH)^{-1}\psi$ for some ψ, and so

$$(\lambda - iH_0)(\lambda - iH)^{-1}\psi - \psi = iV(\lambda - iH)^{-1}\psi$$

for all $\psi \in \mathrm{Ran}(\lambda - iH_0) = \mathcal{H}$. $\mathrm{Ran}(\lambda - iH_0)$ is the range of $(\lambda - iH_0)$. But then we have

$$(\lambda - iH)^{-1}\psi - (\lambda - iH_0)^{-1}\psi = (\lambda - iH_0)^{-1} iV(\lambda - iH)^{-1}\psi$$

for all $\psi \in \mathcal{H}$. Here $\mathcal{H}$ is the Hilbert space in question. q.e.d.

Remark 1.11. Let A, B and H be self-adjoint operators on $\mathcal{H}$, and a and b any complex numbers. Suppose $\overline{A}(\varphi)(t) = \langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$, and $\overline{B}(\varphi)(t) = \langle Be^{-itH}\varphi, e^{-itH}\varphi\rangle$. Suppose each of these functions is differentiable at t. Then $\overline{(aA+bB)}(\varphi)(t)$ is differentiable and $\overline{(aA+bB)}'(\varphi)(t) = a\overline{A}'(\varphi)(t) + b\overline{B}'(\varphi)(t)$.

Proof. We have

$$\begin{aligned}\overline{(aA+bB)}(\varphi)(t) &= \langle (aA+bB)e^{-itH}\varphi, e^{-itH}\varphi\rangle \\ &= a\langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle + b\langle Be^{-itH}\varphi, e^{-itH}\varphi\rangle \\ &= a\overline{A}(\varphi)(t) + b\overline{B}(\varphi)(t).\end{aligned}$$

But each term on the right is differentiable. q.e.d.

Remark 1.12. We emphasize the fact shown in the proof of Lemma 1.7 that if H is self-adjoint then $\|R(\lambda, iH)\|$ is uniformly bounded on Γ_c.

We generalize this fact as follows.

Lemma 1.13. Let H be a self-adjoint operator and V a closed operator on $\mathfrak{H}$ with $D(H) \subset D(V)$. Let $\varphi \in D(H)$, then $\|VR(\lambda, iH)\varphi\|$ is bounded on Γ_c.

Proof. For $\lambda \in \Gamma_c$ we recall that $\lambda = \pm c + ib$ with $c > 0$ and $b \in (-\infty, \infty)$. We assume first that $\lambda = c + ib$. But we have

$R(\lambda, iH)\varphi = \int_0^\infty e^{-\lambda t} e^{itH} \varphi \, dt$, (see Dunford and Schwartz [1,622]).

Now V is closed, so $VR(\lambda, iH)\varphi = \int_0^\infty e^{-\lambda t} V e^{itH} \varphi \, dt$ by Corollary 1.5 if the integral exists. But,

$$\int_0^\infty e^{-\lambda t} V e^{itH} \varphi \, dt = \int_0^\infty e^{-\lambda t} V(c-iH)^{-1} e^{itH} (c-iH)\varphi \, dt ,$$

since $\varphi \in D(H)$. But $V(c-iH)^{-1}$ is bounded, and so the integrand is continuous in t.

Moreover,

$$\|e^{-\lambda t} V(c-iH)^{-1} e^{itH} (c-iH)\varphi\| \leq e^{-ct} \|V(c-iH)^{-1}\| \, \|(c-iH)\varphi\|$$

$$\leq Me^{-ct} .$$

But this is integrable. Thus $\|VR(\lambda, iH)\varphi\| \leq M \int_0^\infty e^{-ct}dt < \infty$.

For $\lambda = -c + ib$ we note that $R(-\lambda, -iH) = -R(\lambda, iH)$. But then $\|VR(\lambda, iH)\varphi\| = \|VR(-\lambda, -iH)\|$, and so the above argument now applies. q.e.d.

Polynomials P(x)

In this section we shall concern ourselves with the case of A being the maximal multiplication operator determined by the polynomial $P(x)$ in the variable $x = (x_1, \ldots, x_n)$. Therefore we shall assume throughout that the Hilbert space $\mathfrak{H}$ is $L^2(R^n)$. Moreover, H_0 will be the self-adjoint closure of the Laplacian $-\Delta$ defined on $\mathcal{S}$ the space of rapidly decreasing functions on R^n. Throughout, the potential V will be a symmetric operator whose domain contains $\mathcal{S}$ such that $(-\Delta + V)|_{\mathcal{S}}$ has a self-adjoint closure $H = H_0 + \overline{V|_{\mathcal{S}}}$ with $D(H_0) = D(H)$. In consonance with the physical considerations in the introduction we shall refer to H_0 as the free Hamiltonian, and H as the Hamiltonian.

We shall make repeated use of the Fourier transform of functions $\varphi \in L^2(R^n)$. We shall denote the transform by $\mathfrak{F}(\varphi)$ or $\hat{\varphi}$. We shall take as a definition of the transform restricted to $\mathcal{S}$

$$\mathfrak{F}(\varphi)(k) = \int_{R^n} e^{-2\pi i\langle x, k\rangle} \varphi(x)dx .$$

If $x = (x_1, \ldots, x_n)$ and $\alpha = (\alpha_1, \ldots, \alpha_n)$, where α_i is a non-negative integer, then we define $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. Moreover, we set $|\alpha| = \sum_{i=1}^{n} \alpha_i$.

In view of the linearity described in Remark 1.11, we need only study multiplication operators of the form x^α. We set $A = x^\alpha$, and interpret A as the self-adjoint closure of x^α defined on $\mathcal{S}$.

We now set about establishing for A the three properties listed on page 9. We begin with properties 1) and 2).

<u>Remark 1.14.</u> Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ where each α_i is a non-negative integer. Let S^α be the space of functions $f \in L^2(R^n)$ such that for each $\beta \leq \alpha$ (i.e., $\beta_i \leq \alpha_i$), f is in the domain of $\overline{\frac{\partial^\beta}{\partial x}}$, where $\overline{\frac{\partial^\beta}{\partial x}}$ is the closure of $\frac{\partial^\beta}{\partial x}$ defined on $\mathcal{S}$. Here, $\frac{\partial^\beta f}{\partial x}$ means $\frac{\partial^{|\beta|} f}{\partial x_1^{\beta_1} \cdots \partial x_n^{\beta_n}}$. Then S^α is a Banach space in the Sobolev norm given by $\|f\|_{S^\alpha}^2 = \sum_{\beta \leq \alpha} \left\| \overline{\frac{\partial^\beta f}{\partial x}} \right\|_{L^2}^2$. The proof is standard and can be found with slight modification in [2, 323].

<u>Remark 1.15.</u> If $\psi \in D(x^\alpha)$ then $\psi \in D(x^\beta)$ for all $\beta \leq \alpha$.

Note that we shall, from time to time, confuse the operators x^α and $\frac{\partial^\alpha}{\partial x}$ with their closures. It will be clear from the context which is meant. Of course in this case

$D(x^\alpha) = \{f \in L^2(R^n) \mid x^\alpha f \in L^2(R^n)\}$, and $x^\alpha = \overline{x^\alpha|_{\mathcal{S}}}$.

Proof. Let $\psi \in D(x^{\alpha})$, then

$$\int_{R^n} |x^{\alpha}|^2 |\psi|^2 dx = \int_{|x| \leq 1} |x^{\alpha}|^2 |\psi|^2 dx + \int_{|x| > 1} |x^{\alpha}|^2 |\psi|^2 dx .$$

But for $|x| > 1$, $|x^{\beta}| \leq |x^{\alpha}|$, so

$$\int_{R^n} |x^{\beta}|^2 |\psi|^2 dx \leq \int_{|x| \leq 1} |x^{\beta}|^2 |\psi|^2 dx + \int_{|x| > 1} |x^{\alpha}|^2 |\psi|^2 dx < \infty .$$

So, $x^{\beta}\psi \in L^2(R^n)$. q.e.d.

Lemma 1.16. If $\psi \in D(x^{\alpha})$ then $R(\lambda, iH_0)\psi \in D(x^{\alpha})$.

Proof. Note that the operator $i^{|\beta|} \frac{\partial^{\beta}}{\partial x}\Big|_{\mathcal{S}}$ is essentially self-adjoint, and its closure has for its Fourier transform $(2\pi)^{|\beta|} k^{\beta}$.

Now let $\psi \in D(x^{\alpha})$, then there is a sequence $\{\psi_n\} \subset \mathcal{S}$, the space of rapidly decreasing functions, such that $\psi_n \to \psi$, and $x^{\alpha}\psi_n \to x^{\alpha}\psi$ in $L^2(R^n)$, since x^{α} is closed. But,

$$\| x^{\alpha}\psi_n - x^{\alpha}\psi \|^2 = \int_{R^n} |x^{\alpha}|^2 |\psi_n - \psi|^2 dx ,$$

and

$$\| x^{\beta}\psi_n - x^{\beta}\psi \|^2 = \int_{R^n} |x^{\beta}|^2 |\psi_n - \psi|^2 dx$$

$$\leq \int_{|x| \leq 1} |\psi_n - \psi|^2 dx + \int_{|x| \geq 1} |x^{\alpha}|^2 |\psi_n - \psi|^2 dx .$$

Thus, $x^\beta \psi_n \to x^\beta \psi$ in $L^2(R^n)$ for each $\beta \leq \alpha$. But then for all $\beta \leq \alpha$, $\frac{\partial^\beta}{\partial k} \hat{\psi}_n \to (\frac{-1}{2\pi i})^{|\beta|}(x^\beta \hat{\psi})$. But S^α is a Banach space, so $\hat{\psi}_n \to \hat{\psi}$ in S^α. So if $\psi \in D(x^\alpha)$ then $\hat{\psi} \in S^\alpha$.

With this fact we have

$$\mathcal{F}[x^\alpha R(\lambda, iH_0)\psi_n] = (\frac{-1}{2\pi i})^{|\alpha|} \frac{\partial^\alpha}{\partial k}[\frac{1}{\lambda - 4\pi^2 i|k|^2} \hat{\psi}_n]$$

$$= (\frac{-1}{2\pi i})^{|\alpha|} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \frac{\partial^{\alpha-\beta}}{\partial k} \frac{1}{\lambda - 4\pi^2 i|k|^2} \frac{\partial^\beta}{\partial k} \hat{\psi}_n .$$

But for fixed λ each $\frac{\partial^{\alpha-\beta}}{\partial k} \frac{1}{\lambda - 4\pi^2 i|k|^2}$ is a bounded multiplication operator. Moreover $\frac{\partial^\beta}{\partial k} \hat{\psi}_n \to \frac{\partial^\beta}{\partial k} \hat{\psi}$ in $L^2(R^n)$, so $\mathcal{F}[x^\alpha R(\lambda, iH_0)\psi_n]$ converges. But $R(\lambda, iH_0)\psi_n$ converges to $R(\lambda, iH_0)\psi$. Since x^α is closed, $R(\lambda, iH_0)\psi \in D(x^\alpha)$. Indeed we have the useful formula

$$\mathcal{F}[x^\alpha R(\lambda, iH_0)\psi] = (\frac{-1}{2\pi i})^{|\alpha|} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \frac{\partial^{\alpha-\beta}}{\partial k} \frac{1}{\lambda - 4\pi^2 i|k|^2} \frac{\partial^\beta \hat{\psi}}{\partial k} ,$$

and

$$x^\alpha R(\lambda, iH_0)\psi = (\frac{-1}{2\pi i})^{|\alpha|} \sum_{\beta \leq \alpha} (\frac{-1}{2\pi i})^{-|\beta|} \binom{\alpha}{\beta} \mathcal{F}^{-1}[\frac{\partial^{\alpha-\beta}}{\partial k} \frac{1}{\lambda - 4\pi^2 |k|^2}] \mathcal{F}(x^\beta \psi).$$

q. e. d.

Remark 1.17. $\frac{\partial^\gamma}{\partial k} \frac{1}{\lambda - 4\pi^2 i|k|^2}$ is a sum of terms of the form $f(k) = C_{a,m} k_1^{a_1} \cdots k_n^{a_n} / (\lambda - 4\pi^2 i|k|^2)^m$ where $|a| < m$ and $|a| \leq |\gamma|$.

Proof. We proceed by induction on $|\gamma|$. If $|\gamma| = 0$ then the assertion is clearly true. Now suppose the assertion is true for $|\gamma| = n$, and

$$f(k) = C_{am} \frac{k_1^{a_1} \cdots k_n^{a_n}}{(\lambda - 4\pi^2 i|k|^2)^m}$$

is one term in the sum. Then

$$\frac{\partial f(k)}{\partial k_i} = C_{am} \frac{a_i k_1^{a_1} \cdots k_i^{a_i - 1} \cdots k_n^{a_n}}{(\lambda - 4\pi^2 i|k|^2)^m} + C'_{am} \frac{k_1^{a_1} \cdots k_i^{a_i + 1} \cdots k_n^{a_n}}{(\lambda - 4\pi^2 i|k|^2)^{m+1}} .$$

Hence the assertion is true for $|\gamma| = n+1$. q.e.d.

We regard $f_\lambda(k) = \frac{k^a}{(\lambda - 4\pi^2 i|k|^2)^m}$, where $|a| \leq 2m$, as a multiplication operator. Since λ will be on Γ_c, $f_\lambda(k)$ is continuous in k, and so the norm of this operator is the supremum of $|f_\lambda(k)|$. We set $g(\lambda) = \operatorname{Sup}_k |f_\lambda(k)|$. The next lemmas show how $g(\lambda)$ behaves as a function of λ on Γ_c.

Lemma 1.18. Let $g(\lambda) = \operatorname{Sup}_k \frac{|k^a|}{|(\lambda - 4\pi^2 i|k|^2)^m|}$ with $\lambda \in \Gamma_c$, and

$|\alpha| \leq 2m$. Then there is a constant $K > 0$ such that
$g(\lambda) \leq K|\lambda|^{|\alpha|/2}$ on Γ_c.

<u>Proof</u>. If $\lambda \in \Gamma_c$ then $\lambda = \pm c + ib$, and so

$$|f_\lambda(k)| = \frac{|k^\alpha|}{(c^2+(b-4\pi^2|k|^2)^2)^{m/2}} .$$

To find the supremum we may as well use the square of this expression,

$$|f_\lambda(k)|^2 = \frac{|k^{2\alpha}|}{(c^2+(b-4\pi^2|k|^2)^2)^m} .$$

Consider k on a sphere of radius r, then $r^2 = \sum_{i=1}^{n} k_i^2$, so $|k_i| \leq r$. Therefore,

$$|f_\lambda(k)|^2 \leq \frac{r^{2|\alpha|}}{[c^2+(b-4\pi^2 r^2)^2]^m} .$$

We shall find the supremum of

$$h_\lambda(r) = \frac{r^{2|\alpha|}}{[c^2+(b-4\pi^2 r^2)^2]^m} .$$

Differentiating we get

$$h'(r) = \frac{\begin{array}{c}[2|\alpha| r^{2|\alpha|-1}(c^2+(b-4\pi^2 r^2)^2)^m \\ +16\pi^2 mr(c^2+(b-4\pi^2r^2)^2)^{m-1}(b-4\pi^2r^2)r^{2|\alpha|}]\end{array}}{[c^2+(b-4\pi^2r^2)^2]^{2m}} .$$

Setting $h'_\lambda(r) = 0$ we get

$$16\pi^4(|\alpha|-2m)r^4 + 8\pi^2(m-|\alpha|)br^2 + |\alpha|(c^2+b^2) = 0 .$$

Now if $|\alpha| = 2m$ and $b \leq 0$ then $h_\lambda(r) \leq \frac{1}{16\pi^4}$ and is asymptotic to this value. If $b > 0$ then $r^2 = \frac{(c^2+b^2)}{4\pi^2 b}$. For this r then $h_\lambda(r) \leq K(\frac{c^2+b^2}{b})^{|\alpha|}$ for some constant K. If $b > |c|$ then $b > \frac{|\lambda|}{2}$, so $h_\lambda(r) \leq 2K|\lambda|^{|\alpha|}$. If $b \leq |c|$ then the computation

$$h_\lambda(r) = \frac{(\frac{c^2+b^2}{4\pi^2 b})^{|\alpha|}}{[c^2+(b-\frac{(c^2+b^2)}{b})^2]^m}$$

$$\leq K_1(c^2+b^2)^{2m}$$

$$\leq K_2 ,$$

for some positive constants K_1 and K_2, shows that for all $0 < b < |c|$ the supremum of $h_\lambda(r)$ is less than or equal to K_2 or the asymptotic value $\frac{1}{(16\pi^4)^m}$. In any of the above cases then $h_\lambda(r) \leq K|\lambda|^{|\alpha|}$ for some K.

Now if $|a| < 2m$, and $h'_\lambda(r) = 0$, and we set $t = r^2$, then

$$t = \frac{-8\pi^2(m-|a|)b \pm \sqrt{64\pi^4(m-|a|)^2 b^2 - 64\pi^4(|a|-2m)|a|(c^2+b^2)}}{32\pi^4(|a|-2m)} .$$

Now with $|a| < 2m$, $h_\lambda(r) \to 0$ as $r \to \infty$, and $h_\lambda(0) = 0$, so one of these values of t determines a value of r at which $h(r)$ is maximum. Let r_0 be one of these values, then

$$g(\lambda) \le \frac{r_0^{|a|}}{(c^2+(b-4\pi^2 r^2)^2)^{m/2}} \le \frac{r_0^{|a|}}{|c|^m}$$

$$\le \frac{1}{|c|^m}\left[\frac{|\lambda|\,|m-|a|\,| + \sqrt{(m-|a|)^2|\lambda|^2 - |a|(|a|-2m)|\lambda|^2}}{4\pi^2\,|\,|a|-2m|}\right]^{|a|/2}$$

$$\le K|\lambda|^{|a|/2} \qquad \text{for some } K > 0. \qquad \text{q.e.d.}$$

<u>Lemma 1.19.</u> For $|a| \le 2m$ the function $g(\lambda)$ is continuous on Γ_c.

<u>Proof.</u> We have $|f_\lambda(k)| = \dfrac{|k|^a}{(c^2+(b-4\pi^2|k|^2)^2)^{m/2}}$ where $\lambda = \pm c + ib$. We shall show that $|f_\lambda|$ converges to $|f_{\lambda_0}|$ uniformly in $k \in R^n$. Indeed,

$$||f_\lambda(k)|^2 - |f_{\lambda_0}(k)|^2|$$

$$= |k^{2\alpha}| \left| \frac{1}{(c^2+(b-4\pi^2|k|^2)^2)^m} - \frac{1}{(c^2+(b_0-4\pi^2|k|^2)^2)^m} \right|$$

$$= \frac{|k^{2\alpha}|}{(c^2+(b-4\pi^2|k|^2)^2)^m} \left| \frac{(c^2+(b_0-4\pi^2|k|^2)^2)^m-(c^2+(b-4\pi^2|k|^2)^2)^m}{(c^2+(b_0-4\pi^2|k|^2)^2)^m} \right| .$$

Now since $|\alpha| \leq 2m$ the quantity $\dfrac{|k^{2|\alpha|}|}{(c^2+(b-4\pi^2|k|^2)^2)^m}$ is bounded by say C_1 for all $k \in R^n$ and all b such that $|b-b_0| \leq 1$. Moreover $(c^2+(b_0-4\pi^2|k|^2)^2)^m - (c^2+(b-4\pi^2|k|^2)^2)^m$ is a polynomial of degree at most $4m-1$ with coefficients $a_\gamma(b)$ such that $a_\gamma(b) \to 0$ as $b \to b_0$. So for all k with $|k|^2 \geq r_0$, for some r_0,

$$\left| \frac{(c^2+(b_0-4\pi^2|k|^2)^2)^m-(c^2+(b-4\pi^2|k|^2)^2)^m}{(c^2+(b_0-4\pi^2|k|^2)^2)^m} \right| \leq \sum_\gamma |a_\gamma(b)| .$$

But this is as small as we please for b close enought to b_0. Now observe that $|f_\lambda(k)|$ is continuous on $[b_0-1, b_0+1] \times B^{n-1}$, where B^{n-1} is the r_0-ball in R^n. This is a compact set, so $|f_\lambda(k)|$ is uniformly continuous there. But the square root function is uniformly continuous on the non-negative real axis, so $|f_\lambda(k)| = \sqrt{|f_\lambda(k)|^2}$ converges uniformly in k to $|f_{\lambda_0}(k)|$ as $h \to \lambda_0$ on Γ_c.

Now $g(\lambda) = \sup_k |f_\lambda(k)| = \| |f_\lambda| \|_\infty$. But $\| \ \|_\infty$ is continuous, so g is continuous since g is a composition of the continuous maps $\lambda \to |f_\lambda(k)|$, and $\| \ \|_\infty : F \to \operatorname{Sup}_k |F(k)|$. q.e.d.

The reader is reminded that $H = H_0 + V$ where H_0 is the closure of $-\Delta$ on $\mathcal{S}$ the space of rapidly decreasing functions, and V is a symmetric operator such that H is the self-adjoint closure of $-\Delta + V$ on $\mathcal{S}$. We assume $D(H) = D(H_0)$, or equivalently $D(H_0) \subset D(V)$.

<u>Theorem 1.20.</u> Let $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ be a monomial on R^n, and let m be an integer such that $m - \frac{|\alpha|}{2} \geq 1 + \epsilon$ where $\epsilon > 0$. Let $\varphi \in D(H^{m+1})$ and $(aI - iH)^m \varphi \in D(x^\alpha)$, where a is fixed and $\operatorname{Re}(a) \neq 0$. Let V be such that for all $\beta \leq \alpha$, $D(H_0) \subset D(x^\beta V)$. Then, $e^{itH}\varphi \in D(x^\alpha)$ for each real t, and $\|x^\alpha e^{itH}\varphi\|$ is bounded for all t in any finite interval.

<u>Proof.</u> We shall employ Lemma 1.8. As a maximal multiplication operator x^α is closed. We must show that if $\psi = (aI - iH)^m \varphi$, then $x^\alpha R(\lambda, iH)\psi$ is defined, and is continuous in λ on Γ_c. Moreover, we must show that $\|x^\alpha R(\lambda, iH)\psi\|$ is of order $|\lambda|^{m-(1+\epsilon)}$ as $|\lambda| \to \infty$.

We have $R(\lambda, iH)\psi = R(\lambda, iH_0)\psi + R(\lambda, iH_0)iVR(\lambda, iH)\psi$. But ψ and $VR(\lambda, iH)\psi \in D(x^\alpha)$, and hence both are in $D(x^\beta)$ for $\beta \leq \alpha$. Then by Lemma 1.16, $R(\lambda, iH)\psi \in D(x^\alpha)$, and

$$x^{\alpha}R(\lambda, iH)\psi = x^{\alpha}R(\lambda, iH_0)\psi + x^{\alpha}R(\lambda, iH_0)iVR(\lambda, iH)\psi$$

$$= \sum_{\beta \leq \alpha} \binom{\alpha}{\beta}\left(\frac{-1}{2\pi i}\right)^{|\alpha|-|\beta|} \mathfrak{F}^{-1}\left[\frac{\partial^{\alpha-\beta}}{\partial k} \frac{1}{\lambda - 4\pi^2 i|k|^2}\right]\mathfrak{F}$$

$$\times \quad [x^{\beta}\psi + x^{\beta} iVR(\lambda, iH)\psi] .$$

But each $B_{\gamma}(\lambda) = \mathfrak{F}^{-1}\left[\frac{\partial^{\gamma}}{\partial k} \frac{1}{\lambda - 4\pi^2 i|k|^2}\right]\mathfrak{F}$ is continuous in λ on Γ_c, and $\|B_{\gamma}(\lambda)\| \leq M_{\gamma}|\lambda|^{|\gamma|/2}$ by Remark 1.17 and Lemmas 1.18 and 1.19. Here $|\gamma| \leq |\alpha|$, so each of the terms $B_{\alpha-\beta}(\lambda)x^{\beta}\psi$ is continuous on Γ_c, and
$\|B_{\alpha-\beta}(\lambda)x^{\beta}\psi\| \leq M_{\alpha-\beta}|\lambda|^{|\alpha|/2}\|x^{\beta}\psi\|$.

In addition each term $x^{\beta}VR(\lambda, iH)\psi$ is continuous in λ on Γ_c, since by the resolvent equation for $\lambda, \mu \in \Gamma_c$

$$x^{\beta}VR(\lambda, iH)\psi - x^{\beta}VR(\mu, iH)\psi = (\mu-\lambda)x^{\beta}VR(\lambda, iH)|(\mu, iH)\psi .$$

Now $R(\mu, iH)\psi \in D(H) \subset D(x^{\beta}V)$, so by Lemma 1.13 $x^{\beta}VR(\lambda, iH)R(\mu, iH)\psi$ is uniformly bounded for $\lambda \in \Gamma_c$ and μ fixed. So $x^{\beta}VR(\lambda, iH)\psi$ is continuous. Moreover, since $\psi \in D(H)$ $x^{\beta}VR(\lambda, iH)\psi$ is uniformly bounded on Γ_c by Lemma 1.13 and the fact that $x^{\beta}V$ is closable. Thus, the terms $B_{\alpha-\beta}(\lambda)x^{\beta} iVR(\lambda, iH)\psi$ are continuous and bounded by some $M'_{\alpha-\beta}|\lambda|^{|\alpha|/2}$ as $|\lambda| \to \infty$ on Γ_c. But then $x^{\alpha}R(\lambda, iH)\psi$ is continuous, and $\|x^{\alpha}R(\lambda, iH)\psi\|$

is of order $|\lambda|^{|a|/2}$. However, $m - \frac{|a|}{2} \geq 1 + \epsilon$, so $\|x^a R(\lambda, iH)\psi\|$ is at most of order $|\lambda|^{m-(1+\epsilon)}$. Thus the theorem follows from Lemma 1.8. q.e.d.

In order to apply Theorem 1.1 we must show that $e^{-itH}\varphi \in D[Hx^a - x^a H]$. But if $H\varphi \in D(H^{m+1})$ and $(aI - iH)^m(H\varphi) \in D(x^a)$ then from Theorem 1.20 we have $e^{-itH}H\varphi \in D(x^a)$. Thus $e^{-itH}\varphi \in D(x^a H)$. Therefore, it remains to find conditions such that $e^{-itH}\varphi \in D(Hx^a)$.

<u>Theorem 1.21.</u> Let m be an integer such that $m - \frac{|a|}{2} \geq 2 + \epsilon$ for some $\epsilon > 0$. Let $\varphi \in D(H^{m+1})$ and $(aI - iH)^m \varphi \in D(x^a)$. Suppose that $D(H_0) \subset D(x^\beta V)$ for all $\beta \leq a$. Then $x^a e^{itH}\varphi \in D(H)$ for all $t \in R$.

<u>Proof</u>. By Theorem 1.20 we have $e^{itH}\varphi \in D(x^a)$. We have the general assumption that $D(H) = D(H_0)$, so we need only show that $x^a e^{itH}\varphi \in D(H_0)$. Therefore, we need only show that $\mathfrak{F}(x^a e^{itH}\varphi) \in D(K^2)$, where $K^2\varphi = |k|^2\varphi$, this being a constant times the Fourier transform of H_0.

We have seen that

$$x^a e^{itH}\varphi = \frac{1}{2\pi i} \int_{\Gamma_c} \frac{e^{\lambda t} x^a R(\lambda, iH)(aI - iH)^m \varphi}{(a-\lambda)^m} \, d\lambda$$

by the hypotheses and the proof of Lemma 1.8. Now $\mathfrak{F}$ is unitary, so

$$\mathfrak{F}(x^\alpha e^{itH}\varphi) = \frac{1}{2\pi i}\int_{\Gamma_c} \frac{e^{\lambda t}\,\mathfrak{F}[x^\alpha R(\lambda, iH)(aI-iH)^m\varphi]}{(a-\lambda)^m}\,d\lambda .$$

As in the proof of Theorem 1.20 we see that if $\psi = (aI-iH)^m\varphi$ then

$$\mathfrak{F}(x^\alpha R(\lambda, iH)\psi) = \sum_{\beta\leq\alpha} \binom{\alpha}{\beta}\left(\frac{-1}{2\pi i}\right)^{|\alpha|}\left[\frac{\partial}{\partial k}^{\alpha-\beta}\frac{1}{\lambda-4\pi^2 i|k|^2}\right]$$
$$\times\left[\frac{\partial}{\partial k}^{\beta}\hat{\psi} + \frac{\partial}{\partial k}^{\beta}(iVR(\lambda, iH)\psi)^\wedge\right].$$

We observe that since $VR(\lambda, iH)\psi \in D(x^\beta)$, $(VR(\lambda, iH)\psi)^\wedge \in D(\frac{\partial}{\partial k}^{\beta})$. But each $\frac{\partial}{\partial k}^{\alpha-\beta}\frac{1}{\lambda-4\pi^2 i|k|^2}$ is a sum of terms of the form $\frac{k^\eta}{(\lambda-4\pi^2 i|k|^2)^P}$ with $|\eta| < P$ by Remark 1.17. So if we multiply by $|k|^2$ we get

$$|k|^2\mathfrak{F}(x^\alpha R(\lambda, iH)\psi) = \sum_{\beta\leq\alpha}\binom{\alpha}{\beta}\left(\frac{-1}{2\pi i}\right)^{|\alpha|}\sum_\gamma \frac{k^\gamma}{(\lambda-4\pi^2 i|k|^2)^{P_\gamma}}$$
$$\times\left[\frac{\partial}{\partial k}^{\beta}(\psi + iVR(\lambda, iH)\psi)^\wedge\right],$$

where $|\gamma| \leq P_\gamma + 1 \leq 2P_\gamma$. But the operators

$$B_\gamma(\lambda) = \frac{k^\gamma}{(\lambda - 4\pi^2 i |k|^2)^{P_\gamma}}$$

are bounded and continuous in norm on Γ_c. Moreover, $\|B_\gamma(\lambda)\| \leq M_\gamma |\lambda|^{|\gamma|/2}$, where $|\gamma| \leq |\alpha| + 2$, (see Remark 1.17 and Lemma 1.18). Thus $\| |k|^2 \mathfrak{F}(x^\alpha R(\lambda, iH)\psi\| \leq c|\lambda|^{(|\alpha|/2)+1}$. But, $m - \frac{|\alpha|}{2} - 1 \geq 1 + \epsilon$, so the integral

$$\int_{\Gamma_c} \frac{e^{\lambda t} K^2 \mathfrak{F}[x^\alpha R(\lambda, iH)(aI - iH)^m \varphi]}{(a-\lambda)^m} d\lambda$$

exists. Consequently Corollary 1.5 implies that $\mathfrak{F}(x^\alpha e^{itH}\varphi) \in D(K^2)$, and so $x^\alpha e^{itH}\varphi \in D(H)$. q.e.d.

<u>Theorem 1.22.</u> Let $P(x)$ be a polynomial of degree r. Let m be an integer such that for some $\epsilon > 0$, $m - \frac{r}{2} \geq 2 + \epsilon$. Let $H = H_0 + V$, and φ be a state such that $\varphi \in D(H^{m+1})$, and $(aI - iH)^{m+1}\varphi \in D(x^\alpha)$ for all $|\alpha| \leq r$. Let the potential V be such that $D(H_0) \subset D(x^\alpha V)$ for all $|\alpha| \leq r$. Then,

$$\overline{P(x)}(\varphi)(t) = \langle P(x) e^{itH}\varphi, e^{itH}\varphi \rangle$$

is differentiable and

$$\overline{P}'(x)(\varphi)(t) = \langle i[HP(x) - P(x)H] e^{itH}\varphi, e^{itH}\varphi \rangle .$$

<u>Proof.</u> By Theorems 1.1, 1.20 and 1.21 the result is true for x^α

with $|\alpha| \leq r$. So by Remark 1.11 the result follows for $P(x)$.

q.e.d.

Potentials and States

In the above theorem it is clear that the hypotheses can be satisfied for a large class of potentials and states. Moreover, the choice of V restricts the choice of φ to some extent, and vice versa. However, from a physical point of view it is more likely that the potential would be determined a-priori, and so we take the point of view that the states are to be determined after a potential is given.

The time is ripe to give sufficient conditions under which our blanket hypotheses on $H = H_0 + V$ hold. Recall that we have assumed that H is self-adjoint and $D(H) = D(H_0)$.

Definition 1.23. Let T and V be operators on some Hilbert space $\mathcal{H}$. V is relatively T-bounded if an only if $D(T) \subset D(V)$ and there are non-negative numbers a and b such that for every $\varphi \in D(T)$

$$\|V\varphi\| \leq a\|\varphi\| + b\|T\varphi\|.$$

The relative T-bound of V is the infimum of all such b.

Theorem 1.24. Let T be essentially self-adjoint. If V is symmetric and relatively T-bounded with bound less than 1, then $T + V$ is essentially self-adjoint and the closure $\overline{(T+V)} = \overline{T} + \overline{V}$.

The proof may be found in [3, 288].

In the case $H = H_0 + V$ where $H_0 = \overline{-\Delta|_{\mathcal{S}}}$ on R^3 and V is a multiplication operator it is enough if $V = V_1 + V_2$ with $V_1 \in L^2(R^3)$ and $V_2 \in L^\infty(R^3)$ [3, 302]. In this case the fact that $D(H_0) \subset D(V)$ depends on the fact that in dimension three the elements of $D(H_0)$ are bounded and continuous. Again this may be found in [3, 302].

Corollary 1.25. Let $P(x)$ be a polynomial of degree r in $x \in R^n$. Let m be the least integer strictly greater than $2 + \frac{r}{2}$. Let $H = H_0 + V$ where $H_0 = \overline{-\Delta|_{\mathcal{S}}}$ and V is a real C^∞ function on R^n with $x^\alpha V$ bounded for all α such that $|\alpha| \leq r$. Moreover, suppose that $\left|\frac{\partial^\alpha V}{\partial x}\right| \leq C_\alpha(1+|x|^2)^{k_\alpha}$ for $|\alpha| \leq 2m$, where C_α and k_α are constants. Let $\varphi \in \mathcal{S}$ the space of rapidly decreasing functions. Then $\overline{P(x)}'(\varphi)(t)$ exists, and $\overline{P(x)}'(\varphi)(t) = \langle i[HP(x)-P(x)H]e^{-itH}\varphi, e^{-itH}\varphi\rangle$.

Proof. V is a bounded operator so Theorem 1.24 applies. Now if $\varphi \in \mathcal{S}$ then $\varphi \in D(H^{m+1})$ and $(aI-iH)^m\varphi \in \mathcal{S}$. But $\mathcal{S} \subset D(x^\alpha)$ for all $|\alpha| \leq r$. But $D(H_0) \subset D(x^\alpha V)$, and $m - \frac{r}{2} \geq 2 + \epsilon$ for some $\epsilon > 0$. Hence the result follows by Theorem 1.22. q.e.d.

The Polynomials $P(\partial/\partial x)$

In this section we study the constant coefficient partial differential operator $P(\frac{\partial}{\partial x})$ where P is a polynomial. The investigation follows similar lines as the foregoing. We therefore consider the operators $i^{|\alpha|}\frac{\partial^\alpha}{\partial x}$ on $\mathcal{S}$ and their self-adjoint closures A^α.

We set $H = H_0 + V$ where $H_0 = \overline{-\Delta|_{\mathcal{S}}}$ and V is a closed symmetric operator such that H is self-adjoint and $D(H) = D(H_0)$.

Theorem 1.26. Suppose $D(H_0) \subset D(A^\alpha V)$. Let $(aI-iH)^2\varphi \in D(A^\alpha)$ and $\varphi \in D(H^3)$. Then $e^{itH}\varphi \in D(A^\alpha)$ for each real t and $\|A^\alpha e^{itH}\varphi\|$ is bounded for all real t in a finite interval.

Proof. Let $\psi = (aI-iH)^2\varphi$ then $\psi \in D(H)$. Observe that A^α permutes with $R(\lambda, iH_0)$. But then we have
$A^\alpha R(\lambda, iH)\psi = R(\lambda, iH_0)A^\alpha\psi + R(\lambda, iH_0)iA^\alpha VR(\lambda, iH)\psi$, since $\psi \in D(A^\alpha)$ and $R(\lambda, iH)\psi \in D(H_0)$. Now since $A^\alpha V$ is closable and $\psi \in D(H)$, $A^\alpha VR(\lambda, iH)\psi$ is continuous and bounded in norm on Γ_c by Lemma 1.13. But $R(\lambda, iH_0)$ is bounded in norm and continuous on Γ_c. Thus, we can apply Lemma 1.8. q.e.d.

Recall again that H permutes with e^{itH}, so if $H\varphi \in D(H^3)$ or $\varphi \in D(H^4)$ and $(aI-iH)^2H\varphi \in D(A^\alpha)$ then
$e^{itH}H\varphi = He^{itH}\varphi \in D(A^\alpha)$. So in order to show that

$e^{itH}\varphi \in D[HA^{\alpha} - A^{\alpha}H]$ it remains to show when $A^{\alpha}e^{itH}\varphi \in D(H)$.

Theorem 1.27. Let $H = H_0 + V$, and suppose $D(H_0) \subset D(A^{\alpha}V)$. Let $\varphi \in D(H^3)$ and $(aI-iH)^2\varphi \in D(A^{\alpha})$. Then, $A^{\alpha}e^{itH}\varphi \in D(H)$.

Proof. We set $\psi = (aI-iH)^2\varphi$, and as before $A^{\alpha}R(\lambda, iH)\psi = R(\lambda, iH_0)A^{\alpha}\psi + R(\lambda, iH_0)iA^{\alpha}VR(\lambda, iH)\psi$. But H_0 is a closed operator and it is easy to see that $H_0R(\lambda, iH_0)$ is bounded for all λ on Γ_c. Indeed,

$$\mathcal{F}\,[H_0R(\lambda, iH_0)]\,\mathcal{F}^{-1} = \frac{4\pi^2|k|^2}{\lambda - 4\pi^2 i|k|^2},$$

and so by Lemma 1.19 $H_0R(\lambda, iH_0)$ is also continuous in λ on Γ_c. Hence $H_0A^{\alpha}R(\lambda, iH)\psi$ is defined and is a continuous and bounded function of λ on Γ_c. But then

$$\int_{\Gamma_c} e^{\lambda t}\,\frac{H_0A^{\alpha}R(\lambda, iH)(aI-iH)^2\varphi}{(a-\lambda)^2}\,d\lambda$$

exists, and so $A^{\alpha}e^{itH}\varphi \in D(H_0) = D(H)$ by Corollary 1.5. q.e.d.

Theorem 1.28. Let P be a polynomial of degree r on R^n. Let φ be a state such that $\varphi \in D(H^4)$ and $(aI-iH)^2\varphi \in D(A^{\alpha})$ for all α such that $|\alpha| \leq r$. For all $|\alpha| \leq r$ let $D(H_0) \subset D(A^{\alpha}V)$. Then for every real t $\overline{P(\frac{\partial}{\partial x})(\varphi)(t)}$ is differentiable and

$$\overline{P(\frac{\partial}{\partial x})}'(\varphi)(t) = \langle i[HP(\frac{\partial}{\partial x}) - P(\frac{\partial}{\partial x})H]e^{-itH}\varphi, e^{-itH}\varphi\rangle .$$

Here

$$P(\frac{\partial}{\partial x}) = \sum_{|\alpha| \leq r} C_\alpha A^\alpha .$$

Proof. This result is an immediate corollary of Theorems 1.1, 1.26 and 1.27. q.e.d.

It should be noted that the hypotheses here have little chance of being satisfied if $|\alpha| > 2$ and V is a multiplication operator since we require $D(H_0) \subset D(A^\alpha V)$. So even if V is smooth we are asking for twice differentiable functions to be differentiable to a higher order. But if V is say an integral operator whose effect is to smooth L^2 functions then the hypotheses can be satisfied. We shall treat the case where $A^\alpha = \frac{\partial}{\partial x_j}$ in Chapter II.

II. APPLICATIONS

In this chapter we shall give sufficient conditions under which Ehrenfect's theorem holds. In addition we shall examine the behavior of the mean of position $\bar{x}_j(\varphi)(t)$ as it relates to the choice of initial state φ.

Ehrenfest's Theorem

We have seen in the introduction that the classical formulas, $m\frac{dx_j}{dt}$ = momentum and $m\frac{d^2x_j}{dt^2}$ = force, have, according to Ehrenfest, an analog in the quantum setting. Indeed, Ehrenfest's theorem in physics [9, 455] asserts that the same formulas hold if x_j is replaced by its mean value as a function of time, and the momentum and force are replaced by their mean values.

Just as in Chapter I we shall assume that $H = H_0 + V$ where H_0 is the free Hamiltonian on $L^2(R^n)$ and V is a potential such that H is self-adjoint and $D(H_0) = D(H)$.

Theorem 2.1. Let x_j be the j-th coordinate operator on $L^2(R^n)$. Let $H = H_0 + V$, with V a multiplication operator, and let φ be such that $\varphi \in D(H^4)$ and $(aI-iH)^4\varphi \in D(x_j)$. Let $D(x_jV) \supset D(H_0)$. Then $\bar{x}_j'(\varphi)(t)$ exists and

$$\bar{x}_j'(\varphi)(t) = \langle i[H_0x_j - x_jH_0]e^{-itH}\varphi, e^{-itH}\varphi\rangle .$$

Proof. In Theorem 1.22 set $r = 1$ and $m = 3$. Observe that $x_j V = V x_j$ on the intersection of their domains. q.e.d.

The Coulomb Potential on $L^2(R^3)$

In $L^2(R^3)$ the Coulomb potential V is given by $V(x) = \frac{1}{|x|}$. Observe that $V \in L^2(R^3)$, and so V satisfies our blanket requirements that $H = H_0 + V$ be self-adjoint with $D(H) = D(H_0)$ so that $D(H_0) \subset D(V)$. Moreover, $|x_j V| = \frac{|x_j|}{|x|} \leq 1$, so $x_j V$ is bounded and $D(H_0) \subset D(x_j V)$.

Let $\mathcal{S}_0$ be the subspace of $\mathcal{S}$ consisting in all those functions $\varphi \in \mathcal{S}$ that vanish in a neighborhood of the origin.

Definition 2.2. Let A be an operator on a Hilbert space $\mathcal{H}$. Then $\varphi \in \mathcal{H}$ is said to be an analytic vector for A if and only if there is a $t > 0$ such that

$$\sum_{n=0}^{\infty} \frac{\|A^n \varphi\| t^n}{n!} < \infty .$$

Theorem 2.3 (Nelson [4, 572]). If A is a symmetric operator on $D(A)$, and if $D(A)$ contains a dense set of analytic vectors then A is essentially self-adjoint.

Lemma 2.4. Consider $\overline{i\frac{\partial}{\partial x_j}}$ as the self-adjoint realization of

$i \frac{\partial}{\partial x_j}$ on $\mathcal{S}$. Then $i(Hx_j - x_jH) \subset \overline{2i \frac{\partial}{\partial x_j}}$.

Proof. One easily calculates that $i(Hx_j - x_jH)$ is symmetric on $D[Hx_j - x_jH]$. Also, for $\varphi \in \mathcal{S}$, $i(Hx_j - x_jH)\varphi = i(H_0x_j - x_jH_0)\varphi = 2i \frac{\partial \varphi}{\partial x_j}$. Now let $A = i(Hx_j - x_jH)$ and $B = i(Hx_j - x_jH)|_{\mathcal{S}} = 2i \frac{\partial}{\partial x_j}$, then both are symmetric operators with $B \subset A \subset \overline{A}$. Now B (hence A) contains a dense set of analytic vectors. Indeed, consider $\frac{\partial}{\partial x_j}$ in the Fourier transform representation. Let $\hat{\varphi} \in C_c^\infty$ with support in a ball of radius R. Then

$$\|k_j^m \hat{\varphi}\| = \left(\int_{L^2(R^n)} |k_j^m|^2 |\hat{\varphi}|^2 dk \right)^{1/2} \leq R^m \|\hat{\varphi}\|.$$

But $\mathcal{F}^{-1}[C_c^\infty R^n)]$ is dense in $L^2(R^n)$, and for $0 < t < \frac{1}{R}$, and $\varphi \in \mathcal{F}^{-1}(C_c^\infty)$, so we have

$$\sum_{n=0}^{\infty} \frac{\|A^n \varphi\| t^n}{n!} \leq \sum_{n=0}^{\infty} \frac{R^n \|\varphi\| t^n}{n!} \leq \|\varphi\| \sum_{n=0}^{\infty} \frac{1}{n!} < \infty.$$

Thus, by Nelson's theorem A is essentially self-adjoint. So, since $B \subset \overline{A}$, $\overline{B} \subset \overline{A}$, so $A \subset \overline{A} \subset \overline{B}$, by taking adjoints.

q.e.d.

Corollary 2.5. Let V be the Coulomb potential then for all $\varphi \in \mathcal{S}_0$, $\overline{x}_j'(\varphi)(t) = <\overline{2i \frac{\partial}{\partial x_j}} e^{-itH}\varphi, e^{-itH}\varphi>$.

Proof. Since $\varphi \in \mathcal{S}_0$, $H\varphi = H_0\varphi + V\varphi \in \mathcal{S}_0$. So by repetition $H^m\varphi \in \mathcal{S} \subset D(x_j)$ for $m \leq 4$. So by Theorem 2.1 and the fact that x_jV is bounded we have $\bar{x}_j'(\varphi)(t) = \langle i[Hx_j - x_jH]e^{-itH}\varphi, e^{-itH}\varphi\rangle$. But by Lemma 2.4 we have

$$\bar{x}_j'(\varphi)(t) = \langle \overline{2i\frac{\partial}{\partial x_j}}\, e^{-itH}\varphi, e^{-itH}\varphi\rangle . \qquad \text{q.e.d.}$$

This corollary says that the velocity of the mean is the mean of momentum. This is the first of the two assertions of Ehrenfest's theorem. It is unfortunate that we cannot continue with the Coulomb potential beyond this point, because the composition $\frac{\partial}{\partial x_j} \circ V$ is not defined on all of $D(H_0)$. We shall therefore turn our attention to smooth potentials.

The Case of Smooth Potentials

In this section we shall assume that $V \in C^\infty(R^n)$ and is a real valued function on R^n such that V, x_jV and $\frac{\partial}{\partial x_j}$ are bounded. Therefore, $H = H_0 + V$ is self-adjoint and $D(H_0) = D(H)$, by Theorem 1.24.

Remark 2.6. $(\overline{\frac{\partial}{\partial x_j}}) \circ V$ is defined on $D(H_0)$.

Proof. Let $\varphi \in \mathcal{S}$ then $\frac{\partial}{\partial x_j}(V\varphi) = \frac{\partial V}{\partial x_j}\varphi + V\frac{\partial \varphi}{\partial x_j}$. Now if

$\varphi \in D(H_0)$ then $\varphi \in D(\overline{\frac{\partial}{\partial x_j}})$ and so there is a sequence $\{\varphi_n\} \subset$

$\varphi_n \to \varphi$ and $\frac{\partial \varphi_n}{\partial x_j} \to \overline{\frac{\partial \varphi}{\partial x_j}}$. But, $V\varphi_n \to V\varphi$ and

$\frac{\partial V\varphi_n}{\partial x_j} \to \frac{\partial V}{\partial x_j}\varphi \to V\overline{\frac{\partial \varphi}{\partial x_j}}$, so $\varphi \in D(\overline{\frac{\partial}{\partial x_j}} \circ V)$ since $\overline{\frac{\partial}{\partial x_j}}$ is closed.

Indeed for $\varphi \in D(H_0)$ we have the formula

$$\overline{\frac{\partial}{\partial x_j}}(V\varphi) = \frac{\partial V}{\partial x_j}\varphi + V\overline{\frac{\partial \varphi}{\partial x_j}}. \qquad \text{q.e.d.}$$

Now observe that since V is smooth the requirements that $\varphi \in D(H^4)$ and $(aI-iH)^4\varphi \in D(x_j)$ are satisfied if $H^m\varphi \in D(x_j)$ for $0 \leq m \leq 4$.

<u>Corollary 2.7</u>. Let φ be a state such that $H^m\varphi \in D(x_j)$ for $0 \leq m \leq 4$. Then $\overline{x}_j'(\varphi)(t) = \langle 2i\overline{\frac{\partial}{\partial x_j}} e^{-itH}\varphi, r^{-itH}\varphi\rangle$.

We now consider the second derivative of the mean. Since $\frac{\partial V}{\partial x_j}$ is bounded $\overline{\frac{\partial}{\partial x_j}} \circ V$ is defined on $D(H_0)$ by Remark 2.6. Consequently from Theorem 1.28 we have the following corollary.

<u>Corollary 2.8.</u> Let V be a real C^∞ potential on R^n with x_jV and $\frac{\partial V}{\partial x_j}$ bounded. Let φ be a state such that $H^m\varphi \in D(x_j)$ for all $0 \leq m \leq 4$, and $H^m\varphi \in D(\overline{\frac{\partial}{\partial x_j}})$ for $m \leq 2$. Then

$$\overline{x}_j''(\varphi)(t) = -2\langle [H\overline{\frac{\partial}{\partial x_j}} - \overline{\frac{\partial}{\partial x_j}}H]e^{-itH}\varphi, e^{-itH}\varphi\rangle .$$

Lemma 2.9.

$$H \overline{\frac{\partial}{\partial x_j}} - \overline{\frac{\partial}{\partial x_j}} H \subset -\frac{\partial V}{\partial x_j}.$$

Proof. On $C_c^\infty(R^n)$ the operator $H \overline{\frac{\partial}{\partial x_j}} - \overline{\frac{\partial}{\partial x_j}} H$ agrees with $-\frac{\partial V}{\partial x_j}$ by the product rule for differentiation. Moreover, these operators are symmetric. Set $A = H \overline{\frac{\partial}{\partial x_j}} - \overline{\frac{\partial}{\partial x_j}} H$ and $B = -\frac{\partial V}{\partial x_j}\Big|_{C_c^\infty}$. Then $B \subset A$. We claim that $C_c^\infty(R^n)$ is a dense set of analytic vectors for B (hence A). Indeed, if $\varphi \in C_c^\infty(R^n)$ then $A^m\varphi \in C_c^\infty(R^n)$ and has support inside that of φ. So

$$\| A^m\varphi\| \subset \| (\frac{\partial V}{\partial x_j})^m \varphi\| \leq \| \frac{\partial V}{\partial x_j} \|^m \|\varphi\|.$$

So

$$\sum_{m=0}^{\infty} \frac{\|A^m\varphi\| t^m}{m!} < \infty$$

for some $t > 0$. So by Nelson's theorem A and B are essentially self-adjoint. Hence $B \subset \bar{A}$, so $\bar{B} \subset \bar{A}$, and so by taking adjoints we have $A \subset \bar{A} \subset \bar{B}$. q.e.d.

Corollary 2.10 (Ehrenfest). Let V be a C^∞ potential with x_jV and $\frac{\partial V}{\partial x_j}$ bounded. Let φ be a state such that $H^m\varphi \in D(x_j)$ for $m \leq 4$ and $H^m\varphi \in D(\overline{\frac{\partial}{\partial x_j}})$ for $m \leq 2$, then

1) $\bar{x}_j'(\varphi)(t) = \langle 2i \frac{\overline{\partial}}{\partial x_j} e^{-itH}\varphi, r^{-itH}\varphi\rangle$, and

2) $\bar{x}_j''(\varphi)(t) = 2\langle \frac{\partial V}{\partial x_j} e^{-itH}\varphi, e^{-itH}\varphi\rangle$.

Proof. Use Corollaries 2.7, 2.8 and Lemma 2.9. q.e.d.

Remark 2.11. Corollary 2.10 is true for any state $\varphi \in \mathcal{S}$ provided the derivatives of V up to order six are of polynomial growth.

The Behavior of the Mean

The Bohr model of the hydrogen atom suggests that the electron can be in two different types of state, either orbitting the nucleus or free. If we assume that eigenstates are orbital states and absolutely continuous states are free states, then we can conjecture that the mean of an eigenstate is constant, and that the mean of an absolutely continuous state goes to infinity as time increases. In this application we shall study these possibilities.

Definition 2.12. Let E be the spectral measure of the self-adjoint operator H on some Hilbert space $\mathcal{H}$. Then we define three subspaces of $\mathcal{H}$ as follows:

1) $\mathcal{H}_{pt}(H) = \sum_{\lambda \in R} \oplus \; E\{\lambda\}\mathcal{H}$, this is called the point space of H.

2) $\mathcal{H}_s(H) = \{\varphi \in \mathcal{H} \mid \langle E(\ )\varphi, \varphi\rangle$ is singular with respect to Lebesgue measure$\}$, this is called the singular space of H.

3) $\mathcal{H}_{ac}(H) = \{\varphi \in \mathcal{H} \mid \langle E(\ )\varphi, \varphi\rangle$ is absolutly continuous with respect to Lebesgue measure$\}$, this is called the absolutely continuous space.

All of these spaces are closed, and in particular $\mathcal{H}_{pt} \subset \mathcal{H}_s$, and $\mathcal{H} = \mathcal{H}_s \oplus \mathcal{H}_{ac}$.

4) We set $\sigma_{pt}(H) = \{\lambda \in R \mid E\{\lambda\} \neq 0\}$, this is called the point spectrum of H. It is well known that for separable Hilbert spaces $\sigma_{pt}(H)$ is countable. Moreover $\sigma_{pt}(H)$ is the set of eigenvalues of H. It is also not difficult to see that $\mathcal{H}_{pt}(H) = E\{\sigma_{pt}(H)\}$.

<u>Remark 2.13</u>. Let $\mathcal{H}$ be any Hilbert space and A and H self-adjoint operators on $\mathcal{H}$. Let φ be an eigenvector of H, $\varphi \in D(A)$ then $\bar{A}(\varphi)(t) = \langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$ is constant.

<u>Proof</u>. Let λ_0 be the eigenvalue of φ then it is well known that $e^{-itH}\varphi = e^{-it\lambda_0}\varphi$. Consequently $e^{-itH}\varphi \in D(A)$. Thus $\bar{A}(\varphi)(t) = \langle Ae^{-it\lambda_0}\varphi, e^{-it\lambda_0}\varphi\rangle$ is constant. q.e.d.

We can say a little more than this.

<u>Theorem 2.14.</u> Let $\mathcal{H}$ be a separable Hilbert space with H and

A self-adjoint operators on $\mathcal{H}$. Let A be defined on every eigenvector of H. Let $\{\varphi_k\}$ be an orthonormal basis of eigen-vectors for $\mathcal{H}_{pt}(H)$. Let $\varphi = \sum_{k=1}^{\infty} a_k \varphi_k$ be such that $\sum_{k=1}^{\infty} |a_k|$ and $\sum_{k=1}^{\infty} |a_k| \, \|A\varphi_k\|$ converge. Then,

1) $e^{itH}\varphi \in D(A)$ for all t, and

2) $\bar{A}(\varphi)(t) = \langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$ is bounded for all t.

Proof. Let

$$e^{itH}\psi_n = e^{itH}\sum_{k=1}^{n} a_k\varphi_k = \sum_{k=1}^{n} a_k e^{it\lambda_k}\varphi_k ,$$

then

$$Ae^{itH}\psi_n = \sum_{k=1}^{n} a_k e^{it\lambda_k} A\varphi_k \to \sum_{k=1}^{\infty} a_k e^{it\lambda_k} A\varphi_k$$

since

$$\sum_{k=1}^{\infty} |a_k e^{it\lambda_k}| \, \|A\varphi_k\|$$

converges. But A is closed, so $e^{itH}\varphi \in D(A)$, and

$$Ae^{itH}\varphi = \sum_{k=1}^{\infty} a_k e^{it\lambda_k} A\varphi_k .$$

Now

$$<Ae^{itH}\varphi, e^{itH}\varphi> = <\sum_{k=1}^{\infty} a_k e^{it\lambda_k} A\varphi_k, \sum_{n=1}^{\infty} a_n e^{it\lambda_n}\varphi_n>$$

$$= \sum_{n=1}^{\infty}\sum_{k=1}^{\infty} a_k \bar{a}_n e^{it(\lambda_k - \lambda_n)} <a\varphi_k, \varphi_n> .$$

Thus,

$$|<Ae^{itH}\varphi, e^{itH}\varphi>| \leq \sum_{n=1}^{\infty}\sum_{k=1}^{\infty} |a_k|\,|a_n|\,\|A\varphi_k\|$$

$$\leq \sum_{n=1}^{\infty} |a_n| \sum_{k=1}^{\infty} |a_k|\,\|A\varphi_k\| < \infty. \qquad \text{q.e.d.}$$

<u>Example 2.15.</u> In order to show that Theorem 2.14 is not vacuous we again study the free Hamiltonian perturbed by the Coulomb potential. In order to get a point spectrum we insist that the potential be attractive. Thus we consider the self-adjoint closure H of $-\Delta - V$ where $V = \frac{1}{|x|}$ on R^3.

It is well known that the point spectrum consists in the eigenvalues $\lambda_n = \frac{C}{n^2}$ for $n = 1, 2, 3 \ldots$. Moreover, it is also well known that, in spherical coordinates, a basis of eigenstates for the point space $\mathcal{H}_{pt}(H)$ is given by the functions

$$\psi_{n\ell m}(r, \theta, \phi) = C_1\left[\frac{(n+\ell)!}{n!(n-\ell-1)!(2\ell+1)!}\right]^{1/2} R_{n\ell}(r) Y_\ell^m(\theta, \phi) .$$

Here, $R_{n\ell}(r)$ has the form $r^{\ell} e^{-C_2/n^r} P_{n'}(r)$ where $P_{n'}(r)$ is a polynomial of degree n' such that $\ell + 1 - n = n'$. The functions $y_{\ell}^{m}(\theta, \phi)$ are the usual spherical harmonics. We also have the conditions that $n = 1, 2, 3, \ldots$, $\ell = 0, 1, 2, \ldots, n-1$, and $m = -\ell, \ldots, 0, \ldots, \ell$. For a discussion of these facts see [5, 164].

Now C_2 is positive so the functions $\psi_{n\ell m}$ decrease rapidly. If A is the multiplication operator $A\varphi = r\varphi$, we see that each $\psi_{n\ell m} \in D(A)$. Thus the hypotheses of Theorem 2.14 are easily satisfied in a practical situation.

The Absolutely Continuous States

We have conjectured that $\mathcal{H}_{ac}(H)$ is the subspace of states for which the mean of position is unbounded. In this section we shall show that under certain conditions this is the case.

Our approach will be to compare the mean of position in the case $H = H_0 + V$ with the mean in the case $H = H_0$ as $t \to \pm\infty$. It is natural in this context to compare $e^{itH}\varphi$ and $e^{itH_0}\varphi$ as $t \to \pm\infty$ as these quantities play a central role in the definition of the respective means. We are therefore led in a reasonable way to a consideration of the wave operators.

The Wave Operators

The behavior of $e^{itH}\varphi$ for large t may be discovered by comparing it with the behavior of the well known quantity $e^{itH_0}\psi$. We would say the two quantities are close if they are asymptotic.

Definition 2.16. We shall say that $\psi \in D(W_{\pm})$ and that $W_{\pm}\psi = \varphi$ if and only if $\|e^{-itH}\varphi - e^{-itH_0}\psi\| \to 0$ as $t \to \infty$ or $t \to -\infty$. But this is equivalent to $\|\varphi - e^{itH}e^{-itH_0}\psi\| \to 0$. Again, equivalently $W_{\pm} = S - \lim_{t \to \pm\infty} e^{itH}e^{-itH_0}$, where $S - \lim$ denotes the strong limit. For heuristic reasons it is clear that the wave operators as defined above are very unlikely to exist if $\psi \in \mathcal{H}_{pt}(H_0)$, many of these states corresponding to bound states physically. So we shall define $W_{\pm}$ only for states $\varphi \in \mathcal{H}_{ac}(H_0)$ such that $W_{\pm}\varphi = \lim_{t \to \pm\infty} e^{itH}e^{-itH}\varphi$ exists. It is easy to show that the domains of $W_{\pm}$ are closed linear subspaces of $\mathcal{H}_{ac}(H_0)$, and that $W_{\pm}$ are bounded operators. We must therefore provide sufficient conditions that $D(W_{\pm}) = \mathcal{H}_{ac}(H_0)$.

Lemma 2.17 ([3, 533]). Let D be a subset of $\mathcal{H}_{ac}(H_0)$ such that the closure of the span of D is $\mathcal{H}_{ac}(H_0)$. Suppose that for each $\varphi \in D$ there is a real s such that $e^{-itH_0}\varphi \in D(H_0) \cap D(H)$ for $s \leq t < \infty$, $(H-H_0)e^{-itH_0}\varphi$ is continuous in t, and $\|(H-H_0)e^{-itH_0}\varphi\|$ is integrable on (s, ∞). Then W_+ exists. A similar result holds for W_- with the obvious modification.

Proof. If $\varphi \in D$ we have $\frac{d}{dt}(e^{itH}e^{-itH_0}\varphi) = ie^{itH}(H-H_0)e^{-itH_0}\varphi$, and this derivative is continuous by hypothesis. Thus, if $W(t) = e^{itH}e^{-itH_0}$ then

$$W(t'')\varphi - W(t')\varphi = i\int_{t'}^{t''} e^{itH}(H-H_0)e^{-itH_0}\varphi\, dt ,$$

so

$$\|W(t'')\varphi - W(t')\varphi\| \leq \int_{t'}^{t''} \|(H-H_0)e^{-itH_0}\varphi\| dt .$$

But by the integrability condition $W(t)$ is seen to be Cauchy, so $W_+\varphi$ exists. But then since W_+ is continuous on D and $D(W_+)$ is a closed linear subspace of $\mathcal{H}_{ac}(H_0)$ the result holds for all $\varphi \in \mathcal{H}_{ac}(H_0)$. q.e.d.

Corollary 2.18 ([3, 535]). Let H_0 be the free Hamiltonian on $L^2(R^3)$ and $H = H_0 + V$ where V is real valued and $V = V_1 + V_2$ with $V_1 \in L^2(R^3)$ and V_2 bounded. Suppose that

$$\int_{R^3} (1+|x|)^{-1+\epsilon}|V(x)|^2 dx < \infty \quad \text{for some} \quad \epsilon > 0.$$

Then $W_\pm$ exist.

We remark that the wave operators do not exist for the Coulomb potential.

We introduce at this point a few facts from Richard Lavine's paper [6, 368].

Definition 2.19. We set $A(t) = e^{itH} A e^{-itH}$ where H is the Hamiltonian $H = H_0 + V$ on $L^2(R^n)$ and A is a suitable operator. Let Q be the projection of $L^2(R^n)$ on $\mathcal{H}_{ac}(H)$. Let $P_i = i \frac{\overline{\partial}}{\partial x_i}$ be the i-th coordinate momentum operator. Let f be a bounded complex valued continuous function on R^n. We define $A = f(P_1, \ldots, P_n)$ by considering its Fourier transform to be the multiplication operator $f(k_1, \ldots, k_n)$.

We say that H satisfies the weak scattering axiom two (w.s.2) if and only if for every $A = f(P_1, \ldots, P_n)$ $S - \lim_{t \to \pm\infty} A(t)Q$ exist.

Lemma 2.20 (Lavine). Assume that $V(H_0+i)^{-1}$ is compact. If A is a possibly unbounded operator whose domain contains $D(H_0)$, and $A(H_0+i)^{-1}$ is bounded, (which is true if A is closed), and $S - \lim_{t \to \pm\infty} [A(H_0+i)^{-1}](t)Q = B_\pm$ exist, then for all $\psi \in D(H)$, $\lim_{t \to \pm\infty} A(t)Q\psi = B_\pm(H+i)\psi$.

Proof. We remark first that if K is a compact operator then $\lim K(t)Q\varphi = 0$. Indeed, $\|K(t)Q\varphi\| = \|Ke^{-itH}Q\varphi\|$. Since $Q\varphi \in \mathcal{H}_{ac}(H)$,

$$<e^{-itH}Q\varphi, \psi> = \int_R e^{-it\lambda} d<E(\ )Q\varphi, \psi> = \int_R e^{-it\lambda} hd|\mu|$$

where $\mu(\ ) = \langle E(\ )Q\varphi, \psi\rangle$. But $|\mu|$ is absolutely continuous with respect to Lebesgue measure, so by the Riemann-Lebesgue lemma $\langle e^{-itH}Q\varphi, \psi\rangle \to 0$ as $t \to \pm\infty$. So $e^{-itH}Q\varphi$ is weakly convergent to zero, and since K is compact $Ke^{-itH}Q\varphi$ is strongly convergent to zero.

Now let $\psi \in D(H)$ and $\varphi = (H+i)\psi$. Then

$$\|A(t)Q(\psi) - B_\pm(H+i)\psi\| = \|A(t)(H+i)^{-1}Q\varphi - B_\pm\varphi\|$$

$$\leq \|A(t)[\{(H+i)^{-1} - (H_0+i)^{-1}\}(t)]Q(\varphi)\|$$

$$+ \|A(t)(H_0+i)^{-1}(t)Q(\varphi) - B_\pm\varphi\| .$$

Now the second term goes to zero by hypothesis. But the first term is the same as $\|[A(t)(H_0+i)^{-1}(t)][V(t)(H+i)^{-1}Q]\varphi\|$. But this last term has the form $\|K(t)Q\varphi\|$ for a compact operator K. So the term goes to zero. q.e.d.

<u>Corollary 2.21</u> (Lavine). Let $P_j = i\frac{\overline{\partial}}{\partial x_j}$. Suppose that H satisfies w.s.2 and $V(H_0+i)^{-1}$ is compact. Then for all $\psi \in D(H)$ $\lim_{t\to\pm\infty} P_j(t)Q\psi$ exist.

<u>Proof</u>. We apply the above lemma with $A = P_j$. Observe that $D(H) = D(H_0)$, since $V(H_0+i)^{-1}$ is compact. Moreover, $D(H_0) \subset D(A)$, and $A(H_0+i)^{-1}$ is bounded. But,

$S - \lim_{t \to \pm\infty} [A(H_0+i)^{-1}](t)Q$ exists, since

$[A(H_0+i)^{-1}](t) = e^{itH} A(H_0+i)^{-1} e^{-itH}$ and $A(H_0+i)^{-1}$ is a continuous function of $P_1, \ldots, P_n$. But w.s.2 is satisfied so

$S - \lim_{t \to \pm\infty} [A(H_0+i)^{-1}(t)Q$ exist. So the result follows from Lemma 2.20. q.e.d.

We remark that $W_\pm$ are complete if and only if

$\text{Ran } W_\pm = \mathcal{H}_{ac}(H)$.

<u>Remark 2.22.</u> If the wave operators $W_\pm$ of $H = H_0 + V$ exist and are complete then H satisfies w.s.2.

<u>Proof</u>. Let $A = f(P_1, \ldots, P_n)$ where f is a bounded, complex continuous function on R^n. Then A commutes with e^{itH_0}. But.

$A(t)Q = e^{itH} A e^{-itH} Q = e^{itH} e^{-itH_0} A e^{itH_0} e^{-itH} Q$, and so

$S - \lim_{t \to \pm\infty} A(t)Q$ exist. q.e.d.

We note that in R^3 with $H = H_0 + V$ the free Hamiltonian perturbed by a potential $V \in L^1 \cap L^2$ the wave operators $W_\pm$ are complete [3, 546].

<u>Remark 2.23</u>. We note that for $V(H_0+i)^{-1}$ to be compact it is enough that V be a real function with V locally square integrable and $V(x) \to 0$ as $|x| \to \infty$, for $n \leq 3$. See [10, 109].

We are now ready for our results on the unboundedness of the mean of position for absolutely continuous states.

Theorem 2.24. Let B_+ be as in Lemma 2.20 where $A = i\overline{\frac{\partial}{\partial x_j}}$. Let $H = H_0 + V$ be such that H satisfies w.s.2 and $V(H_0+i)^{-1}$ is compact. Let x_j be the usual j-th coordinate operator on $L^2(R^n)$. Let $D(H_0) \subset D(x_j V)$. Let φ be a state such that $\varphi \in D(H^4)$ and $H^m\varphi \in D(x_j)$ for $m \leq 4$, and $\varphi \in \mathcal{H}_{ac}(H)$. Suppose that $<B_+(H+i)\varphi, \varphi> \neq 0$. Then $\overline{x}_j(\varphi)(t) \to \pm\infty$ as $t \to +\infty$.

Proof. Since $V(H_0+i)^{-1}$ is compact we have $D(H) = D(H_0)$. By Corollary 2.21 and Lemma 2.20

$$\lim_{t\to\infty} <e^{itH} i \overline{\frac{\partial}{\partial x_j}} e^{-itH}\varphi, \varphi> = <B_+(H+i)\varphi, \varphi> = c$$

which is not zero by hypothesis. But by Theorem 2.1 and Lemma 2.4 $\overline{x}_j'(\varphi)(t) = <2i\overline{\frac{\partial}{\partial x_j}} e^{-itH}\varphi, e^{-itH}\varphi>$. Thus, $\overline{x}_j'(\varphi)(t) \to c$ as $t \to \infty$. Suppose $c > 0$ then for $t > t_0$ $\overline{x}_j'(\varphi)(t) > \frac{c}{2} > 0$. Hence $\overline{x}_j(\varphi)(t) \to \infty$ as $t \to \infty$ by the mean value theorem.

Similarly if $c < 0$ then $\overline{x}_j(\varphi)(t) \to -\infty$. q.e.d.

Corollary 2.25. Let B_+ be as in Lemma 2.20. Let $V(H_0+i)^{-1}$ be compact, and $D(H_0) \subset D(x_j V)$. Let φ be a state such as in Theorem 2.24 above. Suppose also that the wave operator W_+ exists, is complete, and $\varphi = W_+\psi$ for some ψ. Suppose $<i\overline{\frac{\partial\psi}{\partial x_j}}, \psi> \neq 0$.

Then $\bar{x}_j(\varphi)(t) \to \pm\infty$ as $t \to \infty$.

<u>Proof</u>. We must show that $<B_+(H+i)\varphi, \varphi> \neq 0$.

$$<B_+(H+i)\varphi,\varphi> = \lim_{t\to+\infty} <e^{itH}\frac{\partial}{\partial x_j}(H_0+i)^{-1}e^{-itH}(H+i)\varphi,\varphi>$$

$$= \lim_{t\to+\infty} <\frac{\partial}{\partial x_j}(H_0+i)^{-1}e^{itH_0}e^{-itH}(H+i)\varphi, e^{itH_0}e^{-itH}\varphi>$$

$$= <\frac{\partial}{\partial x_j}(H_0+i)^{-1}W_+^*(H+i)\varphi, W_+^*\varphi>,$$

this last since $\frac{\partial}{\partial x_j}(H_0+i)^{-1}$ is bounded. Now $(H+i)\varphi \in \text{Ran } W_+$ since $\text{Ran } W_+$ reduces H the operator W_+^* is intertwining. Thus $W_+^*(H+i)\varphi = (H_0+i)W_+^*\varphi$, (see Theorem 3.2 [3, 529]). So

$$<B_+(H+i)\varphi,\varphi> = <\frac{\partial}{\partial x_j}W_+^*\varphi, W_+^*\varphi> = <\frac{\partial}{\partial x_j}\psi,\psi>.$$

Now Theorem 2.24 applies. q.e.d.

Entirely similar results may be given for $t \to -\infty$ using B_- and W_-.

III. BOUNDED OBSERVABLES

In this chapter we present a few results on the differentiability of bounded observables. This added condition on the observables will enable us to weaken the hypotheses of some of the theorems as our first theorem shows.

Theorem 3.1. Let A be a bounded operator and H a self-adjoint operator on a Hilbert space $\mathcal{H}$. Let $\varphi \in \mathcal{H}$ and $e^{-it_0H}\varphi \in D[HA-AH]$, and $\bar{A}(\varphi)(t) = \langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle$. Then $\bar{A}'(\varphi)(t)$ exists and $\bar{A}'(\varphi)(t_0) = \langle i[HA-AH]e^{-it_0H}\varphi, e^{-it_0H}\varphi\rangle$.

Proof. Without loss of generality we may assume that $t_0 = 0$, for otherwise we replace φ by $e^{-it_0H}\varphi$ in the following argument.

$$\bar{A}'(\varphi)(0) = \lim_{t\to 0} \frac{\langle Ae^{-itH}\varphi, e^{-itH}\varphi\rangle - \langle A\varphi, \varphi\rangle}{t}$$

$$= \lim_{t\to 0} \frac{\langle e^{itH}Ae^{-itH}\varphi - e^{itH}e^{-itH}A\varphi, \varphi\rangle}{t}$$

$$= \lim_{t\to 0} \frac{\langle Ae^{-itH}\varphi - e^{-itH}A\varphi, e^{-itH}\varphi\rangle}{t}$$

$$= \lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - A\varphi - [e^{-itH}A\varphi - A\varphi]}{t}, e^{-itH}\varphi\right\rangle$$

$$= \lim_{t\to 0} \left\langle \frac{Ae^{-itH}\varphi - A\varphi}{t}, e^{-itH}\varphi\right\rangle - \lim \left\langle \frac{e^{-itH}A\varphi - A\varphi}{t}, e^{-itH}\varphi\right\rangle.$$

But A is bounded so

$$\overline{A}'(\varphi)(0) = \langle -iAH\varphi, \varphi\rangle + \langle iHA\varphi, \varphi\rangle$$

$$= \langle i[HA-AH]\varphi, \varphi\rangle \,. \qquad \text{q.e.d.}$$

Note that we have no need of any symmetry condition on A. For differentiability we require only that $e^{-it_0H}\varphi \in D[HA-AH]$.

We now give a criterion of differentiability which is of greater utility.

<u>Theorem 3.2.</u> Suppose A is bounded, $H = H_0 + V$, with V symmetric, H_0 self-adjoint, and V relatively H_0-bounded with bound less than one. Suppose $A(D(H_0)) \subset D(H_0)$. Then for all $\varphi \in D(H)$ and all t, $\overline{A}(\varphi)(t)$ is differentiable and $\overline{A}'(\varphi)(t) = \langle i[HA-AH]e^{-itH}\varphi, e^{-itH}\varphi\rangle$.

<u>Proof</u>. The hypotheses imply that H is self-adjoint and $D(H) = D(H_0)$. But then $A(D(H)) \subset D(H)$. If $\varphi \in D(H)$ then $e^{-itH}\varphi \in D(H)$ for all t, and so $Ae^{-itH}\varphi \in D(H)$. Then, $e^{-itH}\varphi \in D[HA-AH]$, and so the theorem follows by Theorem 3.1.

q.e.d.

<u>Example 3.3.</u> Consider again the space $L^2(R^3)$ and H_0 the self-adjoint closure of $-\Delta$. Let $H = H_0 + V$ where V is any operator on $L^2(R^3)$ satisfying the hypotheses of Theorem 3.2. We

remind the reader that the Coulomb potential is included. Let $P_j = i\frac{\bar{\partial}}{\partial x_j}$ for $j = 1, 2$ and 3 be the momentum operators on $L^2(R^3)$. Let f be any bounded, complex, measurable function on R^3, and define $A = f(P_1, P_2, P_3)$ by $(A\varphi)\ (k_1, k_2, k_3) = f(k_1, k_2, k_3)\varphi$. Then A is bounded. Moreover, $A[D(H_0)] \subset D(H_0)$. Hence for every $\varphi \in D(H)$, $\bar{A}'(\varphi)(t)$ exists at all t.

<u>Definition 3.4.</u> We shall say that a bounded operator A is H-differentiable if and only if $\bar{A}(\varphi)(t)$ is differentiable for each $\varphi \in D(H)$ and for each t, and

$$\bar{A}'(\varphi)(t) = \langle i[HA-AH]e^{-itH}\varphi, e^{-itH}\varphi\rangle .$$

It is worth noting that Theorem 3.2 says that if A is H_0-differentiable then for "small" perturbations V, A is H_0+V-differentiable.

The above example suggests a Banach algebra of bounded operators that are H-differentiable.

<u>Theorem 3.5.</u> Let H_0 and H be as in Theorem 3.2. Let

$$\beta = \{A \in B(\mathfrak{H}) \mid AH_0 \subset H_0A\}$$

then β is a B*-algebra of H-differentiable operators.

Proof. If $A \in \beta$ then Theorem 3.2 ensures that A is H-differentiable. Certainly β is an algebra. We must show it is closed under the taking of limits and adjoints.

Suppose $\{A_n\} \subset \beta$ and $A_n \to A$ in the norm topology. Suppose $\varphi \in D(H_0)$, then $A_n\varphi \in D(H_0)$ and $A_n\varphi \to A\varphi$. But $A_n(H_0\varphi) = H_0(A_n\varphi) \to A(H_0\varphi)$, and H_0 is closed. Thus $H_0A\varphi = AH_0\varphi$, and so β is closed.

Suppose $A \in \beta$. Let $\varphi, \psi \in D(H_0)$, so

$$<H_0\psi, A^*\varphi> = <AH_0\psi, \varphi> = <H_0A\psi, \varphi>$$

$$= <\psi, A^*H_0\varphi> .$$

So $A^*\varphi \in D(H_0)$, and $H_0A^*\varphi = A^*H_0\varphi$. So $A^* \in \beta$. q.e.d.

The above example and theorem suggests the following algebra of bounded operators is an algebra of H-differentiable operators.

Theorem 3.6. Let H_0 and $H = H_0 + V$ be self-adjoint operators with V symmetric, and V relatively H_0-bounded with bound less than one. Let f be any bounded Borel measurable function on R. Then $f(H_0)$ is H-differentiable.

Proof. By $f(H_0)$ we mean $\int_R f(\lambda)dE$ where E is the spectral measure of H_0. We need only show that $f(H_0)H_0 \subset H_0f(H_0)$, but this is well known. So the result follows by Theorem 3.2. q.e.d.

Multiplication Operators

We now turn to the question of H-differentiability of multiplication operators. Throughout this section $\mathcal{H} = L^2(R^n)$, and H_0 will be the self-adjoint closure of the Laplacian Δ as usual.

In view of Theorem 3.2 it will be enough to find conditions on a bounded multiplication operator A such that $A[D(H_0)] \subset D(H_0)$. To do this we shall need to make use of a product rule for distributions given in the following lemma.

Lemma 3.7. Suppose $1 < p, q < \infty$, $\frac{1}{p} + \frac{1}{q} = 1$, and $f, D_j f \in L^p(R^m)$, and $g, D_j g \in L^q(R^m)$. Then $D_j(fg) = D_j f)g + f(D_j g)$ ae. Note that the derivatives are in the distribution sense. Moreover, $\int f(D_j g)dx = -\int (D_j f)g\,dx$.

Proof. Choose a molifier ρ, that is $\rho \in C_c^\infty(R^m)$ with $\int \rho\,dx = 1$ and $0 \leq \rho \leq 1$. Let $f_n = f * \rho_{1/n}$ where $\rho_{1/n}(x) = n\rho(nx)$ then $f_n \in C^\infty(R^m) \cap L^p(R^m)$, and $f_n \to f$ in $L^p(R^m)$. Moreover, $D_j f_n = (D_j f) * \rho_{1/n}$ and so $D_j f_n \in L^p(R^m)$ and $D_j f_n \to D_j f$ in $L^p(R^n)$. But $f_n \in C^\infty(R^m)$, so Leibnitz' formula for distributions gives

$$D_j(f_n g) = (D_j f_n)g + f_n(D_j g) .$$

So $D_j(f_n g) \in L^1(R^n)$. Since $f_n g \in L^1(R^n)$ we have

$\int (D_j f_n) g\, dx = -\int f_n (D_j g) dx$. Thus, Holder's inequality shows that $\int (D_j f) g\, dx = -\int f(D_j g) dx$.

Now let $\varphi \in D(R^m)$ ($C^\infty(R^m)$ with compact support). Then $<D_j(fg), \varphi> = -\int fg D_j \varphi\, dx$. But by Leibnitz' formula again $-gD_j\varphi = -D_j(\varphi g) + \varphi D_j g$, so $D_j(\varphi g) \in L^q(R^m)$, and so

$$<D_j(fg), \varphi> = -\int f D_j(\varphi g) dx + \int f(D_j g)\varphi\, dx.$$

But we have seen that

$$-\int f D_j(\varphi g) dx = \int (D_j f) g \varphi\, dx .$$

But φ was arbitrary so

$$D_j(fg) = (D_j f) g + f(D_j g) \quad \text{ae.} \qquad \text{q.e.d.}$$

We remark that $D(H_0)$ is exactly the Sobolev space of all elements of $L^2(R^n)$ whose derivatives up to order two are also in $L^2(R^n)$.

<u>Corollary 3.8.</u> Let $A \in L^2(R^n) \cap L^\infty(R^n)$ and suppose that the distribution derivatives of A up to order two are in $L^2(R^n) \cap L^\infty(R^n)$. Then $A[D(H_0] \subset D(H_0)$.

Proof. If $\varphi \in D(H_0)$ we must show that $A\varphi \in D(H_0)$. $A\varphi \in L^2(R^n)$ and so it is a distribution. Let D^α be a derivative with $|\alpha| \leq 2$. By an immediate extension of Lemma 3.7,

$$D^\alpha(A\varphi) = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} D^{\alpha-\beta} A D^\beta \varphi .$$

But $D^\beta \varphi \in L^2(R^n)$ and $D^{\alpha-\beta}A$ is essentially bounded, so $D^\alpha(A\varphi) \in L^2(R^n)$. Hence $A\varphi \in D(H_0)$. q.e.d.

Theorem 3.9. Let V be a symmetric operator with V relatively H_0-bounded with bound less than one. Let $A \in L^2(R^n) \cap L^1(R^n)$, and suppose the distribution derivatives up to order two are in $L^2(R^n) \cap L^\infty(R^n)$. Then A is $H_0 + V$-differentiable.

Proof. Immediate from Corollary 3.8 and Theorem 3.2. q.e.d.

Application

Suppose $V \in C^\infty(R^n)$ is a smooth potential satisfying the hypotheses of Theorem 3.9. Then the expected value of potential energy at time t is $\overline{V}(\varphi)(t) = \langle Ve^{-itH}\varphi, e^{-itH}\varphi\rangle$. Thus the rate of change of this average exists and is given by

$$\overline{V}'(\varphi)(t) = \langle i[H_0V - VH_0]e^{-itH}\varphi, e^{-itH}\varphi\rangle .$$

Integral Operators

In this section we give a result in which A is an integral operator with kernel $G(x, y)$. We shall find conditions on G so that $A[D(H_0)] \subset D(H_0)$.

Lemma 3.10. Let H_0 be a closed operator, and A a bounded operator on a Hilbert space $\mathcal{H}$. Let C be a dense subspace of $D(H_0)$, and $A(C) \subset D(H_0)$. Suppose $H_0A|_C$ is bounded. Then $A[D(H_0] \subset D(H_0)$.

Proof. Let $\varphi \in D(H_0)$, then there is a sequence $\{\varphi_n\} \subset C$ such that $\varphi_n \to \varphi$. But then $A\varphi_n \to A\varphi$ since A is bounded. But $A\varphi_n \in D(H_0)$, and $H_0A\varphi_n \to \psi$ for some ψ, since H_0A is bounded on C. But H_0 is closed, so $A\varphi \in D(H_0)$ and $H_0A\varphi = \psi$. q.e.d.

In the next Theorem Δ_x is the Laplacian on R^n, and the subscript denotes the variables with respect to which the derivatives are taken.

Theorem 3.11. Let H_0 be the free Hamiltonian on $L^2(R^n)$. Let $H = H_0 + V$, where V is a symmetric operator relatively H_0-bounded with bound less than one. Let A be an integral operator with kernel $G(x, y)$ such that $G(x, y) \in C_0^2(R^{2n})$. Then

A is H-differentiable.

Proof. By Theorem 3.2 we need only show that $A[D(H_0)] \subset D(H_0)$. We apply Lemma 3.10. Let $\varphi \in C_0^\infty(R^n)$ (C^∞-functions with compact support), then $A\varphi = \int_{R^n} G(x,y)\varphi(y)dy$. But $G(x,y)$ has compact so $A\varphi$ has compact support. Moreover, $A\varphi \in C_0^2(R^n)$, so $A\varphi \in D(H_0)$. Next we show that H_0A is bounded on $C_0^\infty(R^n)$. Since $A\varphi \in C_0^2(R^n$,

$$H_0A\varphi = \Delta_x A\varphi = \Delta_x \int_{R^n} G(x,y)\varphi(y)dy = \int_{R^n} (\Delta_x G(x,y))\varphi(y)dy.$$

Thus we have,

$$\|H_0A\varphi\|^2 = \int_{R^n} \left| \int_{R^n} \Delta_x G(x,y)\varphi(y)dy \right|^2 dx$$

$$\leq \int_{R^n} \left(\int_{R^n} |\Delta_x G(x,y)| \, |\varphi(y)| dy \right)^2 dx.$$

But for each x, $\Delta_x G(x,y)$ and φ are in $L^2(R^n)$, so by Holders inequality we have:

$$\left(\int_{R^n} |\Delta_x G(x,y)| \, |\varphi(y)| dy\right)^2 \leq \int_{R^n} |\Delta_x G(x,y)|^2 dy \|\varphi\|^2 .$$

Thus,

$$\|H_0 A\varphi\|^2 \leq \int_{R^n} |\Delta_x G(x,y)|^2 dx dy \|\varphi\|^2 .$$

Hence $H_0 A$ is bounded on $C_0^\infty(R^n)$, and so $A[D(H_0)] \subset D(H_0)$ by Lemma 3.10. Thus A is H-differentiable. q.e.d.

IV. A REAL STONE'S THEOREM

In this chapter we shall prove a spectral theorem for normal operators on a real Hilbert space. Such a theorem has been given for bounded normal operators by R.K. Goodrich [7, 123]. Here we shall treat the bounded and unbounded cases at one stroke, and we shall use a method that makes the results completely natural. In addition we shall provide a functional calculus for unbounded or bounded normal operators, and thence obtain Stone's theorem for real Hilbert spaces. Thus the treatment of the unbounded case and the provision of Stone's theorem extend Goodrich's note.

It is natural to complexify the real Hilbert space; solve our problems in the complexification, and then lower the results to the real Hilbert space.

The Complexification of H

Let H be a real Hilbert space with inner product $(\, , \,)$. We define the complexification H_c of H in the following way. Let $[\varphi, \psi] \in H \times H$ and $a + ib \in \mathbb{C}$ then we set $(a+ib)[\varphi, \psi] = [a\varphi - b\psi, a\psi + b\varphi]$. This yields a complex vector space H_c. We define an inner product on H_c by

$$<[\varphi, \psi], [\zeta, \eta]> = (\varphi, \zeta) - i(\varphi, \eta) + i(\psi, \zeta) + (\psi, \eta).$$

It is easy to verify that H_c, with inner product $<\ ,\ >$, is a complex Hilbert space. Note that $[\varphi, \psi] = [\varphi, 0] + i[\psi, 0]$. Consider the map $\varphi \to [\varphi, 0]$. This map is an isometric imbedding of H in H_c with image $H \times \{0\}$. Indeed, $\|[\varphi, 0]\|^2 = <[\varphi, 0], [\varphi, 0]> = (\varphi, \varphi) = \|\varphi\|^2$. Thus, we shall identify H with the real subspace $H \times \{0\}$ of H_c, so that $\varphi + i\psi = [\varphi, \psi]$. Then as expected $(\varphi_1 + i\psi_1) + (\varphi_2 + \psi_2) = (\varphi_1 + \varphi_2) + i(\psi_1 + \psi_2)$, and $(a+ib)(\varphi + i\psi) = (a\varphi - b\psi) + i(a\psi + b\varphi)$.

We shall use the language of complex numbers in this context where the meaning is clear. For example given $\varphi + i\psi$ we shall refer to φ as the real part and ψ as the imaginary part.

Operators on H_c

Suppose A and B are real operators on H then we shall define an operator $A + iB$ on H_c by

$$(A+iB)(\varphi + i\psi) = (A\varphi - B\psi) + i(A\psi + B\varphi) .$$

Remark 4.1.

1) $A + iB$ is a complex linear operator on H_c.

2) $A + iB$ is bounded if and only if A and B are bounded on H.

3) If $A + iB = A_1 + iB_1$ then $A = A_1$ and $B = B_1$.

Proof.

1) $(A+iB)[\varphi+i\psi+s+it] = (A+iB)[\varphi+s+i(\psi+t)]$

$= A\varphi + As - B\psi - Bt + i(A\psi+At+B\varphi+Bs)$

$= (A+iB)(\varphi+i\psi) + (A+iB)(s+it)$. A similar calculation can be made for scalar multiples.

2) Suppose $A + iB$ is bounded then

$\|(A+iB)\varphi\|^2 = \|A\varphi\|^2 + \|B\varphi\|^2 \leq \|A+iB\|^2\|\varphi\|^2$ so

$\|A\| \leq \|A+iB\|$ and $\|B\| \leq \|A+iB\|$. Conversely, if A and B are bounded then $A + iB$ clearly maps convergent sequences to convergent sequences.

3) If $A + iB = A_1 + iB_1$ then $(A+iB)\varphi = A\varphi + iB\varphi$, and $(A_1+iB_1)\varphi = A_1\varphi + iB_1\varphi$. q.e.d.

A Counter Example. It is very tempting to conjecture that $\|A+iB\|^2 = \|A\|^2 + \|B\|^2$, but this is not so as the following example shows. Let $H_c = ¢^2 = R^2 + iR^2$ and $H = R^2$. Let $A(\varphi_1, \lambda_2) = (\varphi_1, 0)$ and $B(\varphi_1, \varphi_2) = (0, \varphi_2)$. Then $\|A\| = 1$ and $\|B\| = 1$. Now,

$$\|A+iB\| = \sup_{\|\varphi+i\psi\| = 1} \|(A+iB)(\varphi+i\psi)\|$$

$$= \operatorname{Sup} \sqrt{\|A\varphi-B\psi\|^2+\|A\psi+B\varphi\|^2}$$

$$= \operatorname{Sup} \sqrt{\varphi_1^2+\psi_1^2+\varphi_2^2+\psi_2^2} = 1$$

Remark 4.2. Let A and B be bounded operators on H then

1) $\|A+iB\|^2 \leq 2[\|A\|^2+\|B\|^2]$ and

2) $\|A\| \leq \|A+iB\|$ and $\|B\| \leq \|A+iB\|$.

3) $\|A+iB\| \leq \|A\| + \|B\|$.

Proof.

1)
$$\|A+iB\| = \sup_{\|\varphi+i\psi\|=1} \|(A+iB)(\varphi+i\psi)\|$$
$$= \sup \|(A\varphi-B\psi)+i(A\psi+B\varphi)\|$$
$$= \sup \sqrt{\|A\varphi-B\psi\|^2+\|A\psi+B\varphi\|^2}$$

But

$$\|A\varphi-B\psi\|^2 \leq 2[\|A\varphi\|^2 + \|B\psi\|^2],$$

and

$$\|A\psi+B\varphi\|^2 \leq 2[\|A\psi\|^2+\|B\varphi\|^2]$$

by the parallelogram law. Thus

$$\|A+iB\| \leq \sup \sqrt{2[\|A\|^2\|\varphi+i\psi\|^2+\|B\|^2\|\varphi+i\psi\|^2]}$$
$$\leq \sqrt{2[\|A\|^2+\|B\|^2]}.$$

Parts 2) and 3) are obtained by direct computation with the definition of the norm of an operator. q.e.d.

The above considerations raise the question that if E is a bounded operator on H_c are there bounded real operators E_1 and

E_2 such that $E = E_1 + iE_2$. The answer is yes!

<u>Lemma 4.3.</u> Let E be a bounded operator on H_c then there exist unique bounded operators E_1 and E_2 on H such that $E = E_1 + iE_2$.

<u>Proof</u>. Let $\varphi \in H$ then $E\varphi = E_1\varphi + iE_2\varphi$. We claim that $E = E_1 + iE_2$. Indeed,

$$E(\varphi+i\psi) = E\varphi + iE\psi = E_1\varphi + iE_2\varphi + i[E_1\psi+iE_2\psi]$$

$$= (E_1\varphi-E_2\psi) + i(E_1\psi+E_2\varphi) = (E_1+iE_2)(\varphi+i\psi) \ .$$

The linearity of E_1 and E_2 is established by direct calculation.

q.e.d.

We can get the same sort of results for unbounded operators but a little care is required with domains. If A and B are any real operators on H then we can define $A + iB$ on $D(A) \cap D(B) + i(D(A) \cap D(B))$. We note that if A and B have the common dense domain D in H then $A + iB$ is defined on the dense domain $D + iD$ in H_c. Conversely if E is densely defined on H_c with domain D then $D \cap H + i(D \cap H) \subset D$, so we may define E_1 and E_2 as before and get $E_1 + iE_2 \subset E$.

Complexification of a Real Operator

Let A be a normal operator on H, that is let A be closed and densely defined and $AA^* = A^*A$. We define $\bar{A} = A + 0i$, so that $\bar{A}(\varphi+i\psi) = A\varphi + iA\psi$. We note that in the bounded case $\|\bar{A}\| = \|A\|$.

Lemma 4.4. If A is normal then so is $\bar{A}$.

Proof. $\bar{A}$ is densely defined. Next $\bar{A}$ is closed for if $\varphi_n + i\psi_n \to \varphi + i\psi$ and $A\varphi_n + iA\psi_n \to p + iq$ then $A\varphi = p$ and $A\psi = q$. Now we show that $\bar{A}(\bar{A})^* = (\bar{A})^*\bar{A}$. We may equivalently show that $D(\bar{A}) = D[(\bar{A})^*]$ and $\|\bar{A}(\varphi+i\psi)\| = \|(\bar{A})^*(\varphi+i\psi)\|$ for all $\varphi + i\psi \in D(\bar{A})$. Observe that $p + iq \in D[(\bar{A})^*]$ if and only if $\langle A\varphi+iA\psi, p+iq\rangle = \langle \varphi+i\psi, s+it\rangle$ for all $\varphi + i\psi \in D(\bar{A})$. In which case $(\bar{A})^*(p+iq) = s + it$. But,

$$\langle A\varphi+iA\psi, p+iq\rangle = (A\varphi, p) - i(A\psi, p) + i(A\varphi, q) + (A\psi, q)$$
$$= (\varphi, s) - i(\psi, s) + i(\varphi, t) + (\psi, t).$$

Setting $\psi = 0$ we get $(A\varphi, p) = (\varphi, s)$ and $(A\varphi, q) = (\varphi, t)$, so $p, q \in D(A^*)$ and $A^*p = s$ and $A^*q = t$. But A is normal so $p, q \in D(A)$. Similarly if $p + iq \in D(\bar{A})$ then $p + iq \in D[(\bar{A})^*]$. Indeed we see that $(\bar{A})^* = (\overline{A^*})$. But then

$$\|(\bar{A})^{*}(\varphi+i\psi)\| = \|\overline{(A^{*})}(\varphi+i\psi)\| = \sqrt{\|A^{*}\varphi\|^{2}+\|A^{*}\psi\|^{2}}$$

$$= \sqrt{\|A\varphi\|^{2}+\|A\psi\|^{2}} = \|\bar{A}(\varphi+i\psi)\|. \qquad \text{q.e.d.}$$

Consequently $\bar{A}$ has a spectral representation $\bar{A} = \int_{\mathbb{C}} z dE$, Where E is a projection valued spectral measure on the Borel sets of $\mathbb{C}$. But then we get two operators E_1 and E_2 on H such that $E(\ ) = E_1(\ ) + iE_2(\ )$. If we calculate purely formally we get

$$\bar{A} = \int (x+iy)d(E_1+iE_2)$$

$$= \int x dE_1 - \int y dE_2 + i[\int x dE_2 + \int y dE_1].$$

Therefore, it is completely natural to conjecture that

$$A = \int x dE_1 - \int y dE_2 .$$

<u>A Spectral Theorem for Real Operators</u>

We begin by discussing some of the properties of E_1 and E_2. First E_1 and E_2 are bounded operator valued functions. Indeed they are measures.

We have $E(\phi) = 0 = E_1(\phi) + iE_2(\phi)$, is $E_1(\phi) = E_2(\phi) = 0$. Let $\bigcup_{n=1}^{\infty} M_n$ be a countable disjoint union of Borel sets in $\mathbb{C}$, then

$$E\left(\bigcup_{n=1}^{\infty} M_n\right)\varphi = \sum_{n=1}^{\infty} E(M_n)\varphi = \sum_{n=1}^{\infty} E_1(M_n)\varphi + i\sum_{n=1}^{\infty} E_2(M_n)\varphi$$

$$= E_1\left(\bigcup_{n=1}^{\infty} M_n\right)\varphi + iE_2\left(\bigcup_{n=1}^{\infty} M_n\right)\varphi$$

for any $\varphi \in H$. So

$$E_k\left(\bigcup_{n=1}^{\infty} M_n\right)\varphi = \sum_{n=1}^{\infty} E_k(M_n)\varphi .$$

Moreover, the sum is independent of order of summation. Consequently, for $\varphi, \psi \in H$, $(E_k(\ )\ \varphi, \psi) = \mu_{k,\varphi,\psi}(\ )$ is a real measure for $k = 1, 2$.

We remark that $E_1(\mathbb{C}) = I$ and $E_2(\mathbb{C}) = 0$ since $E(\mathbb{C}) = I = I + i0$.

<u>Remark 4.5.</u> Let E be the spectral measure of $\bar{A}$ and $E = E_1 + iE_2$. Then,

1) E_1 is self-adjoint and E_2 is skew-adjoint.

2) For Borel sets M_1 and M_2,

   a) $E_1(M_1 \cap M_2) = E_1(M_1)E_1(M_2) - E_2(M_1)E_2(M_2)$

   b) $E_2(M_1 \cap M_2) = E_2(M_1)E_1(M_2) + E_1(M_1)E_2(M_2)$

3) For any Borel set M,

a) $E_1(M) = E_1^2(M) - E_2^2(M)$, and

b) $E_2(M) = E_1(M)E_2(M) + E_2(M)E_1(M)$.

Proof. 1) follows from the fact that E is self-adjoint, and the fact that a little computation shows that $E^* = E_1^* - iE_2^*$. The rest follows from the fact that $E(M_1 \cap M_2) = E(M_1)E(M_2)$. q.e.d.

Remark 4.6. For $\varphi \in H$, $(E_1(\ )\varphi, \varphi)$ is a positive measure and $(E_2(\ )\varphi, \varphi) = 0$.

Proof. Note that E_2 is skew-adjoint so $(E_2(\ )\varphi, \varphi) = 0$. Now

$$(E_1(\ )\varphi, \varphi) = (E_1^2(\ )\varphi - E_2^2(\ )\varphi, \varphi)$$

$$= (E_1(\ )\varphi, E_1(\ )\varphi) + (E_2(\ )\varphi, E_2(\ )\varphi) \geq 0 \ . \qquad \text{q.e.d.}$$

Integrals. We shall need to define the operators $\int f(z)dE_k$ where f is a measurable complex valued function on $\mathbb{C}$.

Since $\mu_{k,\varphi,\psi}(\ ) = (E_k(\ )\varphi, \psi)$ is a bounded real valued measure we may define

$$\int f(z)d\mu_{k,\varphi,\psi} = \int f(z)h(z)d|\mu_{k,\varphi,\psi}|$$

where $|\mu_{k,\varphi,\psi}|$ is the total variation of $\mu_{k,\varphi,\psi}$ and h is the Radon-Nikodym derivative of $\mu_{k,\varphi,\psi}$ with respect to $|\mu_{k,\varphi,\psi}|$.

We observe that for any complex measures μ and λ, if f is μ and λ integrable then

$$\int f d(\mu+\lambda) = \int f d\mu + \int f d\lambda$$

We shall also set $\mu_{\varphi,\psi}(\ ) = \langle E(\ )\varphi, \psi\rangle$.

<u>Theorem 4.7.</u> Consider $\mu_{\varphi,\psi}$ and $\mu_{k,\varphi,\psi}$ for $k = 1, 2$ where $\varphi, \psi \in H$. Then, $\mu_{\varphi,\psi} = \mu_{1,\varphi,\psi} + i\mu_{2,\varphi,\psi}$. Moreover, if f is any complex Borel measurable function on $\mathbb{C}$ then f is $\mu_{\varphi,\psi}$-integrable if and only if f is $\mu_{k,\varphi,\psi}$-integrable for $k = 1$ and 2. In this case

$$\int f(z) d\mu_{\varphi,\psi} = \int f(z) d\mu_{1,\varphi,\psi} + \int f(z) d\mu_{2,\varphi,\psi}.$$

<u>Proof.</u> First

$$\begin{aligned} \mu_{\varphi,\psi} &= \langle E(\ )\varphi,\psi\rangle = \langle (E_1(\ )+iE_2(\ ))\varphi,\psi\rangle \\ &= (E_1(\ )\varphi,\psi) + i(E_2(\ )\varphi,\psi) = \mu_{1,\varphi,\psi} + i\mu_{2,\varphi,\psi} . \end{aligned}$$

Now let f be $\mu_{\varphi\psi}$-integrable. But for any Borel measurable set M, $|\mu_{k,\varphi,\psi}(M)| \leq |\mu_{\varphi,\psi}(M)| \leq |\mu_{\varphi\psi}|(M)$. But by the minimum bounding property of total variation we must have

$|\mu_{k,\varphi,\psi}|(M) \leq |\mu_{\varphi\psi}|(M)$, for $k = 1$ and 2. But then f is $\mu_{k,\varphi,\psi}$-integrable.

Conversely if f is $\mu_{k,\varphi,\psi}$-integrable for $k = 1$ and 2, then, since $|\mu_{\varphi,\psi}| \leq |\mu_{1,\varphi,\psi}| + |\mu_{2,\varphi,\psi}|$, f is $\mu_{\varphi,\psi}$-integrable.

q.e.d.

We are now in a position to define the operators $X_k = \int x dE_k$ and $Y_k = \int y dE_k$ for $k = 1,2$. Recall that $E = E_1 + iE_2$ is the spectral measure of $\overline{A} = A + i0$ where A is a normal operator. We shall take as the domain of these operators X_k and Y_k the space $D(A)$. We observe that if $\varphi \in D(A)$ then $\int |x| d|\mu_{\varphi\psi}| \leq \int |z| d|\mu_{\varphi\psi}| < \infty$ for all $\psi \in H$. The same can be said for y, so x and y are both $\mu_{k,\varphi,\psi}$ integrable for all $\psi \in H$ by Theorem 4.7.

We are going to use the Riesz representation theorem to define X_k and Y_k. We would like to define linear functionals by

$$L_{k,\varphi}(\psi) = \int x d(E_k(\ )\varphi, \psi) ,$$

and

$$R_{k,\varphi}(\psi) = \int y d(E_k(\ )\varphi, \psi)$$

on H. Clearly $L_{k,\varphi}$ and $R_{k,\varphi}$ are linear and real valued, and the next theorem establishes the continuity.

<u>Theorem 4.8.</u> For each $\varphi \in D(A)$ and $k = 1$ or 2, $L_{k,\varphi}$ and $R_{k,\varphi}$ are continuous.

<u>Proof</u>. Observe that

$$|L_{k,\varphi}(\psi)| = \left|\int x d(E_k(\ )\varphi, \psi)\right| \leq \int |x| d|\mu_{k,\varphi,\psi}|$$
$$\leq \int |z| d|\mu_{\varphi\psi}| .$$

But from arguments in the complex case we know that

$$\int |z| d|\mu_{\varphi,\psi}| \leq \int |z|^2 d|\mu_{\varphi\varphi}| \, \|\psi\| .$$

Hence, $L_{k,\varphi}$ is continuous, and the same argument may be applied to $R_{k,\varphi}$. q.e.d.

Thus we may write $L_{k,\varphi}(\psi) = (X_k\varphi, \psi)$, and $R_{k,\varphi}(\psi) = (Y_k\varphi, \psi)$, by the Riesz representation theorem. Clearly X_k and Y_k are linear on $D(A)$.

<u>Theorem 4.9</u> (The Spectral Theorem). Let A be a densely defined normal operator on H, and let $E = E_1 + iE_2$ be the spectral measure of $\bar{A}$, then $A = \int x dE_1 - \int y dE_2 = X_1 - Y_2$.

<u>Proof</u>. For $\varphi, \psi \in D(A)$ we have

$$<\overline{A}\varphi, \psi> = (A\varphi, \psi) = \int z d<E(\ )\varphi, \psi>$$

$$= \int (x+iy)d(\mu_{1,\varphi,\psi} + i\mu_{2,\varphi,\psi})$$

$$= \int x + iy d\mu_{1,\varphi,\psi} + i \int (x+iy) d\mu_{2,\varphi,\psi}$$

$$= \int x d\mu_{1,\varphi,\psi} - \int y d\mu_{2,\varphi,\psi} ,$$

because $(A\varphi, \psi)$ is real. So

$$(A\varphi, \psi) = (\int x dE_1 \varphi, \psi) - (\int y dE_2 \varphi, \psi)$$

$$= ([\int x dE_1 - \int y dE_2]\varphi, \psi) . \qquad \text{q.e.d.}$$

We emphasize at this point that the above theorem is a special case of the more general problem of defining operators of the form $\int u dE_k$ where u is any real valued Borel measurable function. If u is a bounded real valued function all domain difficulties disappear and we may define $u_k = \int u dE_k$ on all of H. Indeed, we set $(\int u dE_k \varphi, \psi) = \int u d<E_k(\ )\varphi, \psi>$ and argue as before.

Further Properties of E_1 and E_2

In order to establish a uniqueness theorem for the spectral representation of A we need to study E_1 and E_2 more closely.

Let us suppose that A is a bounded normal operator on H, then $\bar{A} = A + i0$ is bounded and normal, and the spectral measure E of $\bar{A}$ is concentrated in a disk D centered at the origin in $\mathbb{C}$. Then from the spectral theorem in the complex case we get $(\bar{A})^n((\bar{A})^*)^m = \int_D z^n \bar{z}^m dE$. But we observe that $(\bar{A})^n((\bar{A})^*)^m = A^n(A^*)^m + i0$. Now a straightforward computation using polar coordinates for convenience, that is $x = r\cos\theta$ and $y = r\sin\theta$, shows that

$$(\bar{A})^n((\bar{A})^*)^m = \int_D r^{n+m}\cos(n-m)\theta dE_1 - \int_D r^{n+m}\sin(n-m)\theta dE_2$$

$$+ i[\int_D r^{n+m}\sin(n-m)\theta dE_1 + \int_D r^{n+m}\cos(n-m)\theta dE_2] .$$

Thus,

$$A^n(A^*)^m = \int_D r^{n+m}\cos(n-m)\theta dE_1 - \int_D r^{n+m}\sin(n-m)\theta dE_2 ,$$

and

$$\int_D r^{n+m}\sin(n-m)\theta dE_1 = - \int_D r^{n+m}\cos(n-m)\theta dE_2 .$$

Lemma 4.10 [7, 123]. If A is a bounded normal operator on the real Hilbert space H, and $S \subset R^2$ is a Borel set, and S^* is the reflection of S across the x-axis, that is $S^* = \{(x, -y) \mid (x, y) \in S\}$, then $E_1(S) = E_1(S^*)$ and $E_2(S^*) = -E_2(S)$.

Proof. If $\varphi \in H$ then $(E_2(\ )\varphi, \varphi) = 0$, since E_2 is skew-adjoint. Therefore $0 = \int_D r^{n+m} \cos(n-m)\theta d(E_2(\ )\varphi, \varphi) = -\int_D r^{n+m} \sin(n-m)\theta d\mu$ where $\mu(S) = (E_1(S)\varphi, \varphi)$, $\varphi \in H$. Let f be continuous on D and $f(r, -\theta) = -f(r, \theta)$. Given $\epsilon > 0$ the Stone-Weierstrass theorem provides a trigonometric polynomial $P(r, \theta)$ such that $|f(r, \theta) - P(r, \theta)| < \frac{\epsilon}{2}$ on D, where

$$P(r, \theta) = \sum a_{nm} r^{n+m} \sin(n-m)\theta + \sum b_{nm} r^{n+m} \cos(n-m)\theta.$$

But $|-f(r, \theta) - P(r, -\theta)| < \frac{\epsilon}{2}$, so $|f(r, \theta) - P(r, \theta) + f(r, -\theta) - P(r, -\theta)| < \epsilon$, and so $|\sum b_{nm} r^{n+m} \cos(n-m)\theta| < \frac{\epsilon}{2}$. But then we must have $|f(r, \theta) - \sum a_{nm} r^{n+m} \sin(n-m)\theta| < \epsilon$. Consequently $\int_D f(r, \theta) d\mu = 0$. If S is a compact set in the upper half plane then there exists a sequence of continuous functions $\{f_n\}$, with $\{f_n\}$ uniformly bounded converging poitwise to χ_S and vanishing off the upper half plane. Here χ_S is the characteristic function of S. Let g_n equal f_n in the upper half plane and equal $-f_n$ in the lower half plane, then $\int g_n d\mu = 0$. But $g_n \to \chi_S - \chi_{S^*}$ pointwise, so by the dominated convergence theorem $\int \chi_S - \chi_{S^*} d\mu = 0$, or $\mu(S) = \mu(S^*)$. Let B be the collection of Borel sets lying in the upper half plane and such that $\mu(S) = \mu(S^*)$. This is easily seen to be a σ-algebra which as we already know contains the compact sets of the upper half plane. Hence B contains all the Borel sets in the upper half plane. But it is then immediate that $\mu(S) = \mu(S^*)$ for every Borel set. Thus, $(E_1(S)\varphi, \varphi) = (E_1(S^*)\varphi, \varphi)$ for all $\varphi \in H$. Now $E_1(S)$ is self-adjoint and so the polarization principle in the complexification gives $(E_1(S)\varphi, \psi) = (E_1(S^*)\varphi, \psi)$, so $E_1(S) = E_1(S^*)$.

Now

$$\int_D r^{n+m} \cos(n-m)\theta dE_2 = - \int_D r^{n+m} \sin(n-m)\theta dE_1,$$

and E_1 is x-axis symmetric, so

$$\int_D r^{n+m} \cos(n-m)\theta d(E_2(\ )\varphi, \psi) = 0.$$

Thus similar arguments give $E_2(S) = -E_2(S^*)$. q.e.d.

Suppose now that A is an unbounded normal operator on H. We shall employ F. Riesz' reduction to the bounded case to show that the above theorem is still true. In what follows we refer the reader to [8, 307 ff].

Lemma 4.11. Let A be an unbounded normal operator on H, and $E = E_1 + iE_2$ the spectral measure of $\bar{A}$. If $S \subset R^2$ is a Borel set and S^* its x-axis reflection, then $E_1(S) = E_1(S^*)$, and $E_2(S) = -E_2(S^*)$.

Proof. Let $\bar{A} = A + i0$ as before, and let $B = (I+(\bar{A})(\bar{A})^*)^{-1}$. B is bounded and self-adjoint, and its corresponding spectral measure F is concentrated in $[0,1]$. Now if $B = C + iD$ then $(C+iD)(I+\bar{A}(\bar{A})^*) = (C+iD)[(I+AA^*)+i0) = I + i0$. Thus $C(I+AA^*) = I$ and $D(I+AA^*) = 0$. But $(I+AA^*)$ is one to one and has a dense range. So $D = 0$. Therefore $B = C + 0i$. But then if $F = F_1 + iF_2$ $F_2 = 0$ by Lemma 4.10. Set $P_n = F(\frac{1}{n+1}, \frac{1}{n})$, as in the reduction to the bounded case, then $P_n : H \to H$; that is, H is invariant under the projection P_n. By reduction to the bounded case we have

$$H_c = \sum_{n=1}^{\infty} \oplus_{\perp} P_n H_c = \sum_{n=1}^{\infty} \oplus_{\perp} H_{cn} = \sum_{n=1}^{\infty} \oplus_{\perp} (H_n + iH_n),$$

where $H_{cn} = P_n H_c$ and $H_n = P_n H$. Moreover we have $\bar{A} = \sum_{n=1}^{\infty} \oplus_{\perp} \bar{A}_n$ and $E = \sum_{n=1}^{\infty} \oplus_{\perp} E_n$ where E_n is the spectral measure of $\bar{A}_n : H_{cn} \to H_{cn}$. Here $\bar{A}_n$ is $\bar{A}|_{H_{cn}}$. Moreover if $A_n = A|_{H_n}$ then $\bar{A}|_{H_{cn}} = \bar{A}_n = A_n + 0i$. But each $\bar{A}_n$ is bounded and normal, so by Lemma 4.10, if $E_n = E_{1n} + iE_{2n}$ then E_{1n}

and E_{2n} satisfy $E_{1n}(S) = E_{1n}(S^*)$ and $E_{2n}(S) = -E_{2n}(S^*)$, $S \subset R^2$. Let $\varphi \in H$, $S \subset R^2$, and $E = E_1 + iE_2$, then

$$E_1(S^*)\varphi = \text{Re } E(S^*)\varphi \quad \text{(the real part)}$$

$$= \text{Re} \sum_{n=1}^{\infty} \oplus_{\perp} E_n(S^*)P_n\varphi = \text{Re} \sum_{n=1}^{\infty} \oplus_{\perp} [E_{1n}(S)P_n\varphi - E_{2n}(S)P_n\varphi]$$

$$= \sum_{n=1}^{\infty} \oplus_{\perp} E_{1n}(S)P_n\varphi.$$

On the other hand

$$E_1(S)\varphi = \text{Re } E(S)\varphi = \sum_{n=1}^{\infty} \oplus_{\perp} E_{1n}(S)P_n\varphi \ ,$$

so $E_1(S) = E_1(S^*)$. Similarly, $E_2(S) = -E_2(S^*)$. q.e.d.

<u>The Uniqueness of E_1 and E_2</u>

<u>Definition 4.12</u> [7, 125]. Let E_1 and E_2 be bounded operator valued measures on the Borel sets of R^2 in the real Hilbert space H. Then (E_1, E_2) is a spectral pair if and only if for S, S_1 and S_2 Borel sets in R^2, and S^* the x-axis reflection of S we have:

1) $E_1(S)$ is self-adjoint and $E_2(S)$ is skew-adjoint,

2) $E_1(S) = E_1(S^*)$, and $E_2(S) = -E_2(S^*)$,

3) $E_1(S_1 \cap S_2) = E_1(S_1)E_1(S_2) - E_2(S_1)E_2(S_2)$, and

$E_2(S_1 \cap S_2) = E_1(S_1)E_2(S_2) + E_2(S_1)E_1(S_2)$, and

4) $E_1(R^2) = I$, and $E_2(R^2) = 0$.

Remark 4.13. If A is normal and $E = E_1 + iE_2$ is the spectral measure of $\bar{A}$ then (E_1, E_2) is a spectral pair.

Theorem 4.14. Let A be a normal operator on a real Hilbert space H, and let (E_1', E_2') be a spectral pair such that $A = \int x dE_1' - \int y dE_2'$. Then $E_1' = E_1$ and $E_2' = E_2$ where $E = E_1 + iE_2$ is the spectral measure of $\bar{A}$.

Proof. Since (E_1', E_2') is a spectral pair the integrals $\int y dE_1'$ and $\int x dE_2'$ are also defined on $D(A)$, the domain of A. Indeed they are both zero. Thus

$$A + i0 = \int x dE_1' - \int y dE_2' + i\left[\int y dE_1' + \int x dE_2'\right]$$

$$= \int (x+iy) dE',$$

where $E' = E_1' + iE_2'$. E' is a spectral measure. Indeed,

$$(E'(S))^2 = (E_1'(S))^2 - (E_2'(S))^2 + i[E_2'(S)E_1'(S) + E_1'(S)E_2'(S)]$$

$$= E_1'(S) + iE_2'(S) = E'(S).$$

Clearly $E'(S)$ is self-adjoint and $E'(R^2) = I$. The strong additivity comes from the strong additivity of the components.

Thus, the uniqueness theorem in the complex case gives $E' = E$. q.e.d.

<u>A Function Calculus for A</u>

Let $f(z) = u(z) + iv(z)$ be a Borel measurable function on R^2. Let $E = E_1 + iE_2$ be the spectral measure of $A + i0 = \bar{A}$, where A is a normal operator on the real Hilbert space H. Assume that f is bounded. Then

$$f(\bar{A}) = \int f(z)dE = \int (u+iv)d(E_1+iE_2)$$

$$= \int udE_1 - \int vdE_2 + i[\int udE_2 + \int vdE_1] .$$

Now if we want $f(\bar{A})$ to be a real operator we must have $\int vdE_1 + \int udE_2 = 0$. But we can achieve this if v is odd with respect to the x-axis and u is even. This is because $E_1(S) = E_1(S^*)$ and $E_2(S) = -E_2(S^*)$.

<u>Remark 4.15.</u> The set of all $f = u + iv$ where f is a bounded Borel measurable function on R^2, and u is even with respect to the x-axis and v is odd is a real algebra. We shall denote this algebra by $\mathcal{A}$.

Definition 4.16. For $f \in \mathcal{A}$ we define

$$f(A) = \int u dE_1 - \int v dE_2 = \int (u+iv) dE|_H .$$

Theorem 4.17. The map $F : \mathcal{A} \to L(H)$, where $L(H)$ is the set of bounded operators on H, defined by $F(f) = f(A)$ is an algebra homomorphism. Moreover, $\bar{f}(A) = (f(A))^*$, where $\bar{f} = u - iv$.

Proof. We have $f(A) = \int f(z) dE|_H$, so the additivity and real scalar multiplication are clear. But from the same result in the complex case

$$f_1 \cdot f_2(A) = \int f_1(z) f_2(z) dE|_H = \int f_1(z) dE|_H \int f_2(z) dE|_H$$
$$= f_1(A) \circ f_2(A) .$$

Also from the complex case we have $\bar{f}(A) = (f(A))^*$. q.e.d.

Stone's Theorem--Real Case

We begin this section with the construction of a particular unitary group on H associated with a given normal operator A on H.

For each real t consider the function

$f_t(z) = \cos(ty) + i \sin(ty)$. Observe that $\cos(ty)$ is even with respect to the x-axis and $\sin(ty)$ is odd. Thus for each t, $f_t \in \mathcal{A}$. Let (E_1, E_2) be the spectral pair of A, and set

$$f_t(A) = \int \cos ty \, dE_1 - \int \sin(ty) dE_2 .$$

<u>Theorem 4.18.</u> $f_t(A)$ is a strongly continuous one parameter unitary group.

<u>Proof.</u> Clearly $f_0(A) = I$. Now

$$\begin{aligned} f_{t_1+t_2} &= \cos(t_1+t_2)y + i \sin(t_1+t_2)y \\ &= \cos t_1 y \cos t_2 y - \sin t_1 y \sin t_2 y \\ &\quad + i[\sin t_1 y \cos t_2 y + \cos t_1 y \sin t_2 y] \\ &= f_{t_1} \cdot f_{t_2} . \end{aligned}$$

Thus, by Theorem 4.17, $f_{t_1+t_2}(A) = f_{t_1}(A) f_{t_2}(A)$. So $f_{-t}(A) = (f_t(A))^{-1}$. But $f_{-t} = \overline{f}_t$, so $(f_t(A))^{-1} = \overline{f}_t(A) = (f_t(A))^*$. Therefore, $f_t(A)$ is a unitary operator on H. We must establish that $f_t(A)$ is strongly continuous. Observe that if $t \to t_0$ then $\cos(t-t_0)y \to 1$ and $\sin(t-t_0)y \to 0$, where the convergence is pointwise. But then

$$\|f_t(A)\varphi - f_{t_0}(A)\varphi\|^2 = (f_t(A)\varphi - f_{t_0}(A)\varphi, f_t(A)\varphi - f_{t_0}(A)\varphi)$$

$$= 2\|\varphi\|^2 - 2(f_t(A)\varphi, f_{t_0}(A)\varphi)$$

$$= 2\|\varphi\|^2 - 2(f_{t-t_0}(A)\varphi, \varphi)$$

$$= 2\|\varphi\|^2 - 2[\int \cos(t-t_0)y d <E_1(\ )\varphi, \varphi>$$

$$- \int \sin(t-t_0)y d <E_2(\ )\varphi, \varphi>] .$$

So by dominated convergence $\|f_t(A)\varphi - f_{t_0}(A)\varphi\| \to 0$. q.e.d.

We are going to show that the unitary group described above is the only one.

Let $u(t)$ be a strongly continuous one parameter group of unitary operators on a real Hilbert space H. We define

$$u'(0)\varphi = \lim_{h \to 0} \frac{u(h)\varphi - \varphi}{h}$$

if the limit exists. We define $D(u'(0)) = \{\varphi \in H \mid u'(0)\varphi \text{ exists}\}$. Certainly $u'(0)$ is an operator on this domain. We shall use the method of complexification again to show that $u'(0)$ is densely defined and skew-adjoint.

<u>Theorem 4.19.</u> Let $u(t)$ be a strongly continuous unitary group

(in brief, a unitary group) on the real Hilbert space H. Let $\bar{u}(t) = u(t) + i0$ be the complexification of $u(t)$. Then

1) $\bar{u}(t)$ is a unitary group on H_c,

2) $D(\bar{u}'(0)) = D(u'(0)) + iD(u'(0))$, and $\bar{u}'(0) = \overline{u'(0)}$, and

3) If u and v are unitary groups and $u'(0) = v'(0)$ then $u = v$.

Proof. 1) If $\bar{u}(t)(\varphi+i\psi) = 0$ then $u(t)\varphi = u(t)\psi = 0$, and so $\varphi = \psi = 0$. Let $\zeta + i\eta \in H_c$ then there exist φ and $\psi \in H$ such that $u(t)\varphi = \zeta$ and $u(t)\psi = \eta$, so $\bar{u}(t)(\varphi+i\psi) = \zeta + i\eta$. Thus $\bar{u}(t)$ is a bijection on H_c. Moreover,

$$\bar{u}(t_1+t_2) = u(t_1+t_2) + i0 = u(t_1)u(t_2) + i0$$

$$= (u(t_1)+i0)(u(t_2)+i0) = \bar{u}(t_1)\bar{u}(t_2) .$$

Finally,

$$\|\bar{u}(t)(\varphi+i\psi)\|^2 = \|u(t)\varphi\|^2 + \|u(t)\psi\|^2 = \|\varphi+i\psi\|^2 .$$

Hence $\bar{u}(t)$ is a unitary group.

2) $$\bar{u}'(0)(\varphi+i\psi) = \lim_{h\to 0} \frac{\bar{u}(h)(\varphi+i\psi)-(\varphi+i\psi)}{h}$$

$$= \lim_{h\to 0} \frac{u(h)\varphi-\varphi}{h} + i \lim \frac{u(h)\psi-\psi}{h}$$

$$= u'(0)\varphi + iu'(0)\psi .$$

So $\varphi + i\psi \in D(\bar{u}'(0))$ if and only if $\varphi + i\psi \in D(u'(0)) + iD(u'(0))$.

3) Suppose u and v are unitary groups on H with $u'(0) = v'(0)$, then $\bar{u}'(0) = u'(0) + iu'(0) = v'(0) + iv'(0) = \bar{v}'(0)$. So by the complex Stone theorem $\bar{u}(t) = \bar{v}(t)$, so $u(t) = v(t)$. q.e.d.

Corollary 4.20. If $u(t)$ is a real unitary group then $u'(0)$ is densely defined.

Proof. $\bar{u}'(0)$ is densely defined, so $D(\bar{u}'(0)) = D(u'(0)) + iD(u'(0))$ is dense. Thus $D(u'(0))$ is dense in H. q.e.d.

Corollary 4.21. $u'(0)$ is skew-adjoint.

Proof. We set $G = u'(0)$ for brevity. By the complex Stone theorem $\bar{G} = G + i0$ is skew-adjoint. We show that $(\bar{G})^* = \overline{G^*}$. Suppose $\varphi + i\psi \in D(\overline{G^*})$ then $\varphi, \psi \in D(G^*)$. Thus for every $\zeta + i\eta \in D(\bar{G})$, $(G\zeta, \varphi) = (\zeta, G^*\varphi)$ and $(G\eta, \psi) = (\eta, G^*\psi)$. But then

$$
\begin{aligned}
\langle \bar{G}(\zeta+i\eta), \varphi+i\psi\rangle &= \langle G\zeta+iG\eta, \varphi+i\psi\rangle \\
&= (G\zeta, \varphi) - i(G\zeta, \psi) + i(G\eta, \varphi) + (G\eta, \psi) \\
&= (\zeta, G^*\varphi) - i(\zeta, G^*\psi) + i(\eta, G^*\varphi) + (\eta, G^*\psi) \\
&= \langle \zeta+i\eta, \overline{G^*}(\varphi+i\psi\rangle
\end{aligned}
$$

Hence, $\overline{G^*} \subset (\bar{G})^*$.

Conversely, if $\varphi + i\psi \in (\bar{G})^*$ then for every $\zeta + i\eta \in D(\bar{G})$ we have,

$$\langle \bar{G}(\zeta+i\eta), \varphi+i\psi\rangle = \langle \zeta+i\eta, (\bar{G})^*(\varphi+i\psi)\rangle$$

$$= \langle \zeta+i\eta, -G\varphi-iG\psi\rangle$$

since $\bar{G}$ is skew-adjoint. Thus

$$\langle \bar{G}(\zeta+i\eta), \varphi+i\psi\rangle = (G\zeta, \varphi) - i(G\zeta, \psi) + i(G\eta, \varphi) + (G\eta, \psi)$$

$$= (\zeta, -G\varphi) - i(\zeta, -G\psi) + i(\eta, -G\varphi) + (\eta, -G\psi).$$

Set $\eta = 0$ to get $(G\zeta, \varphi) = (\zeta, -G\varphi)$ and $(G\zeta, \psi) = (\zeta, -G\psi)$. So $-G\varphi = G^*\varphi$ and $-G\psi = G^*\psi$. So $\varphi + i\psi \in D(\overline{G^*})$, and $(\bar{G})^*(\varphi+i\psi) = \overline{G^*}(\varphi+i\psi)$. So $\overline{G^*} = (\bar{G})^*$, and thus G is easily seen to be skew-adjoint. q.e.d.

Recall the particular unitary group corresponding to the normal operator A on H given by

$$f_t(A) = \int \cos ty \, dE_1 - \int \sin ty \, dE_2.$$

<u>Remark 4.22.</u> Let $u(t)$ be a unitary group on H with infinitesimal generator $u'(0)$. Then the above arguments have shown that the infinitesimal generator of $\bar{u}(t)$ is $\overline{u'(0)}$.

<u>Theorem 4.23.</u> Let A be a skew-adjoint operator on H, then $f_t(A)$ has infinitesimal generator A.

Proof. Observe that

$$\overline{f_t(A)} = f_t(A) + i0$$

$$= \int \cos ty\, dE_1 - \int \sin ty\, dE_2 + i[\int \cos ty\, dE_2 + \int \sin ty\, dE_1]$$

$$= \int e^{ity} d(E_1 + iE_2).$$

Now A is skew-adjoint, so $\bar{A} = A + i0$ is skew-adjoint with spectral measure $E_1 + iE_2$ concentrated on the imaginary axis. But because of this $\bar{A} = \int (x+iy)d(E_1+iE_2) = \int iy\, d(E_1+iE_2)$. Therefore $-i\bar{A}$ is self-adjoint, and $-i\bar{A} = \int yd(E_1+iE_2)$ where we regard $E_1 + iE_2$ as a measure on R. But then if we set $B = -i\bar{A}$ then $e^{itB} = \int e^{ity} d(E_1+iE_2) = \overline{f_t(A)}$. But this implies that $iB = \bar{A}$ is the generator of $\overline{f_t(A)}$. So by the preceding remark $\bar{A} = \overline{(f_t(A)'(0)} = \overline{f_t(A)'(0)} = A + i0$. So A is the infinitesimal generator of $f_t(A)$. q.e.d.

Theorem 4.24. Let $u(t)$ be a unitary group on the real Hilbert space H. Then there exists a unique skew-adjoint operator A such that $u(t) = f_t(A)$.

Proof. By Corollary 4.21 $A = u'(0)$ is skew-adjoint. Set $v(t) = f_t(A)$ then $v'(0) = A$ by Theorem 4.23. So by Theorem 4.19 $u = v$. Suppose now that $u(t) = f_t(B)$ where B is skew-adjoint. Then $u'(0) = B$. q.e.d.

BIBLIOGRAPHY

[1] Dunford, N. and Schwartz, J.T. Linear Operators, Part I: General Theory. Interscience, New York, (1958).

[2] Treves, François. Topological Vector Spaces Distributions and Kernels. Academic Press, New York, (1967).

[3] Kato, Tosio. Perturbation Theory for Linear Operators. Springer-Verlag, New York, (1966).

[4] Nelson, E. Annals of Mathematics, 67, (1959).

[5] Prugovecki, E. Quantum Mechanics in Hilbert Space. Academic Press, New York and London, (1971).

[6] Lavine, R. Journal of Functional Analysis, Vol. 5, No. 3 June, (1970).

[7] Goodrich, R.K. Acta Sci. Math. (Szeged), 33, (1972).

[8] Riesz, F. and Sz-Nagy, B. Functional Analysis. Ungar, New York, (1971).

[9] Ehrenfest, P. Zeitschrift der Physik, 45, (1927).

[10] Rejto, P. Pacific Journal of Math., 19, (1966).