CHAPTER 3 : ONE-PARAMETER UNITARY GROUPS AND FREE PARTICLES

The main purpose of this chapter is to introduce the quantum mechanics of free particles. For this, we first give a general framework to describe a quantum mechanical system, sometimes called the quantum kinematics, and then the dynamics of such a system. Section 3-1 is mathematical in nature and enunciates Stone's theorem for continuous one-parameter unitary groups. In Section 3-2 we briefly sketch the description of a quantum mechanical system in a complex Hilbert space along with some physically motivated examples. Finally Section 3-3 is devoted entirely to studying a particular one-parameter unitary group, viz. the so-called free evolution group and its various ramifications.

3-1 STONE'S THEOREM

Continuous one-parameter unitary groups play very important roles in quantum mechanics. In particular, they are useful to describe the time evolution of quantum mechanical systems, as we shall see in Sections 3-2 and 3-3. Unitary groups arise out of the need to represent symmetry transformations on states of a system, and readers interested in pursuing this question are referred to [P], Wigner [1]. A strongly continuous one-parameter unitary group is defined to be a mapping U from the real line into the set $B(H)$ of all bounded operators on H having the following properties :

(a) strong continuity : $\operatorname*{s-lim}_{\tau\to 0} (U_{t+\tau} - U_t) = 0$ for all $t\varepsilon R$, (3.1)

(b) unitarity : $U_t^* = U_t^{-1}$ for all $t\varepsilon R$, (3.2)

(c) group property : $U_t U_s = U_s U_t = U_{t+s}$, $t,s\varepsilon R$ and $U_o = I$. (3.3)

We shall attempt to justify the continuity property in the next section. It is however important to state here that for a group, strong continuity at any $t\varepsilon R$ is equivalent to strong continuity at $t = 0$, and that for unitary groups, strong continuity is equivalent to weak continuity (Problem 3.1). The main theorem in this section is Stone's theorem which associates a self-adjoint operator with every continuous one-parameter unitary group. The converse of this theorem is also true, viz. that every self-adjoint operator generates a continuous one-parameter unitary group.

PROPOSITION 3.1 : (Stone's Theorem) : Let $\{U_t\}$, $-\infty < t < \infty$,

be a strongly continuous one-parameter unitary group in H. Define a linear operator A (called the <u>infinitesimal generator</u> of $\{U_t\}$) as follows :

$$D(A) = \{f \mid \text{s-lim } i\tau^{-1}(U_\tau - I)f \text{ exists as } \tau \to 0\},$$

and $$Af = \text{s-lim } i\tau^{-1}(U_\tau - I)f \quad \text{for } f \varepsilon D(A). \tag{3.4}$$

Then D(A) is dense and A is self-adjoint.

We give the proof of Stone's theorem in Section 3-4 and that of the converse theorem in Chapter 5. An immediate and interesting consequence of Stone's theorem is the following corollary.

<u>COROLLARY 3.2</u> : (a) Let W be a unitary operator and let U_t, A, D(A) be as in Proposition 3.1. Furthermore, suppose W commutes with U_t for all $t \varepsilon R$. Then W leaves D(A) invariant and

$$WA = AW. \tag{3.5a}$$

(b) In particular, choosing W to be U_t itself, so that the commutation property is trivially satisfied, it follows that U_t leaves D(A) invariant and

$$U_t A = AU_t. \tag{3.5b}$$

<u>Proof</u> : Since W commutes with U_τ, one has

$$Wi\tau^{-1}(U_\tau - I)f = i\tau^{-1}(U_\tau - I)Wf.$$

For all $f \varepsilon D(A)$, the left hand side of the above equation has a strong limit as $\tau \to 0$, viz. WAf. Therefore, by Proposition 3.1, $Wf \varepsilon D(A)$ and the limit of the right hand side is AWf, implying $WD(A) \subseteq D(A)$ and $WA \subseteq AW$. Since $U_t W = WU_t$ implies $W^{-1}U_t = U_t W^{-1}$, identical conclusions are reached with W^{-1} replacing W, i.e. $W^{-1}D(A) \subseteq D(A)$ and $W^{-1}A \subseteq AW^{-1}$.

Upon multiplication by W, one obtains together with the first set of inclusions that $D(A) \subseteq WD(A) \subseteq D(A)$ and $A \subseteq WAW^{-1} \subseteq AWW^{-1} = A$, which shows that all these inclusions must in fact be equalities. #

3-2 DESCRIPTION OF QUANTUM MECHANICAL SYSTEMS

As in classical mechanics, the description of a quantum mechanical system needs two basic physical concepts, that of the states and that of the observables of the system. Such a description can be made conveniently in a Hilbert space, the properties of which we have studied in Chapter 2. Here we shall not give the experimental motivations leading to this Hilbert space structure. Nor shall we describe any other parallel or more basic formalisms of quantum mechanics. For some of these questions the reader is referred to [EM], [M] or [P].

A <u>state</u> of the system is represented by a positive*) trace class operator ρ in H, called the <u>density operator</u> (or density matrix when a specific basis is referred to), which also satisfies $\mathrm{Tr}\,\rho = 1$. For the definition of trace class operators, the reader is referred to Section 2-3. We may deduce that the non-zero spectrum of ρ consists of positive eigenvalues λ_i, satisfying $\sum_i \lambda_i = 1$, where each λ_i is repeated as many times as the multiplicity of the eigenvalue. In the special case $\rho^2 = \rho$, ρ is a projection with one-dimension-

---

*) A linear operator A is said to be <u>positive</u>, written $A \geq 0$, if $(f,Af) \geq 0$ for all $f \in D(A)$.

al range. Such a state is called pure, in contrast with a general density operator ρ which is said to be a mixed state. In this book we shall be concerned almost exclusively with pure states.

If we denote by F_f the projection operator onto the one-dimensional subspace generated by f, then it is clear that to each pure state F_f one may associate a unit ray in H defined by $\{\alpha f \mid |\alpha| = 1\}$, where $\|f\| = 1$. This correspondence between pure states and unit rays is one-to-one. For the purposes of this book, however, we shall identify a pure state with a unit vector in its range, though this is not strictly accurate. For further discussion of this point, the reader should consult [M] or [P].

The observables of the system are represented by self-adjoint operators in H. In the following, we shall identify an observable with its representative self-adjoint operator A in H. In practice, to assign an operator to a given observable, one is guided by physical intuition derived from the corresponding classical problem. However, there are exceptions to this general practice.

The expectation value of an observable A in a pure state f is defined as

$$\mathrm{Exp}_f(A) = (f, Af) \tag{3.6}$$

whenever it exists. In most cases of physical interest, the operator A happens to be unbounded, making $\mathrm{Exp}_f(A)$ undefined whenever $f \notin D(A)$.

As we shall see in Chapter 5, every self-adjoint

operator A admits a spectral resolution, viz. there exists a unique family of projections $\{E_\lambda\}_{\lambda\varepsilon R}$ with the following properties :

(i) $E_\lambda = E_{\lambda+0} = \underset{\eta\to+0}{\text{s-lim}}\, E_{\lambda+\eta}$, *) (3.7)

(ii) $\underset{\lambda\to-\infty}{\text{s-lim}}\, E_\lambda = 0$, $\underset{\lambda\to+\infty}{\text{s-lim}}\, E_\lambda = I$, (3.8)

(iii) If $\lambda \leq \mu$, then $E_\lambda E_\mu = E_\mu E_\lambda = E_\lambda$. (3.9)

(iv) A vector f belongs to D(A) if and only if $\int_{-\infty}^{\infty} \lambda^2 d(f,E_\lambda f) < \infty$,

and for such an f and any $g\varepsilon H$, one has

$$(g,Af) = \int_{-\infty}^{\infty} \lambda\, d(g,E_\lambda f)\ . \tag{3.10}$$

This family of projections $\{E_\lambda\}$ is called the <u>spectral family</u> of the self-adjoint operator A. With the help of the spectral family $\{E_\lambda\}$, one can define a probability measure $p^A_{(a,b],f}$ on R as

$$p^A_{(a,b],f} = \int_a^b d(f,E_\lambda f), \tag{3.11}$$

where $-\infty < a < b < \infty$ and $f\varepsilon H$, $||f|| = 1$. That it is a measure is obvious from the definition, and the fact that

$$p^A_{(-\infty,\infty),f} = \int_{-\infty}^{\infty} d(f,E_\lambda f) = ||f||^2 = 1$$

makes it a probability measure. One interprets $p^A_{(a,b],f}$ as the probability that a measurement of the observable A on the system in the state f will yield a value in the interval (a,b]. This is sometimes known as "Born's probabilistic interpretation" in the quantum mechanics literature and forms

---

*) The notation $\eta\to+0$ means that η tends to zero through positive values.

the basis of all calculations and hence all predictions of the theory. For a state vector $f\varepsilon D(A)$, the expectation value of the observable A in the state f is given by (3.6) and (3.10) as

$$\mathrm{Exp}_f(A) \equiv (f,Af) = \int_{-\infty}^{\infty}\lambda d(f,E_\lambda f) = \int_{-\infty}^{\infty}\lambda\ p^A_{(d\lambda),f} \quad ,$$

which is in conformity with the usual definition of the expectation in probability theory.

Now we give three examples of quantum systems with corresponding Hilbert spaces, states and observables.

<u>Example 3.3</u> : <u>Spinless particle in a box in one dimension</u>.

The relevant Hilbert space is $L^2[a,b]$, i.e. the vector space of the equivalence classes of all Lebesgue measurable complex-valued functions defined on the interval [a,b] which are absolutely square-integrable. The (pure) states of the particle are given by unit vectors $f\varepsilon L^2[a,b]$. One relevant observable is the position which is represented by the operator Q defined as follows :

$$D(Q) = \{f\varepsilon L^2[a,b] \mid \int_a^b |xf(x)|^2 dx < \infty\} \qquad (3.12)$$

and for $f\varepsilon D(Q)$: $(Qf)(x) = xf(x)$. It follows from Proposition 2.16 that Q is a bounded and everywhere defined self-adjoint operator. Its spectral family F_y is given by

$$(F_y f)(x) = \chi_{[a,y]}(x)f(x), \qquad (3.13)$$

where $\chi_I(x)$ is the characteristic function of the interval I. It is easy to verify the properties (3.7) - (3.10) for F_y (Problem 3.2). And the probability that a measurement of the position of the particle in the state f will yield a value in the interval I is given by

$$p^Q_{I,f} = \int_I d(f,F_x f) = \int_I |f(x)|^2 dx. \qquad (3.14)$$

This leads to the commonly found statement that a particle in the state f has position probability density $|f(x)|^2$.

Another observable of physical interest is the momentum P. To define it, we first introduce an operator $\hat{P}$ by

$$\begin{aligned} D(\hat{P}) &= \{f\varepsilon L^2[a,b] \mid f \text{ absolutely continuous}, \\ &\qquad f'\varepsilon L^2[a,b],\ f(a) = f(b) = 0\}, \\ (\hat{P}f)(x) &= -i(h/2\pi)f'(x), \text{ for all } f\varepsilon D(\hat{P}), \end{aligned} \qquad (3.15)$$

where h is Planck's constant. Thus defined, $\hat{P}$ is closed and symmetric but not self-adjoint. In fact it has uncountably many self-adjoint extensions P_ϕ, given by the boundary conditions $f(a) = e^{i\phi}f(b)$, $\phi\varepsilon[0,2\pi]$, as has been pointed out in Section 2-2. The box may be viewed as an apparatus confining the particle to the interval [a,b] and may be used to measure the momentum of the particle. The choice of such an apparatus will determine the boundary condition at the walls of the box and hence the observable P_ϕ (see [P]). For other physical aspects of these observables, see [RO].

<u>Example 3.4</u> : <u>Spinless particle in n-dimensional infinite space</u>.

The Hilbert space of interest here is $L^2(R^n)$ which was introduced in Section 2-1. The (pure) states of the particle are given by unit vectors $f\varepsilon L^2(R^n)$. The position observable is given by an n-component operator $\{Q_j\}_{j=1}^n$ as

$$D(Q_j) = \{f\varepsilon L^2(R^n) \,\Big|\, \int |x_j f(\underline{x})|^2 d^n x < \infty\}$$

and

$$(Q_j f)(\underline{x}) = x_j f(\underline{x}) \text{ for } f \varepsilon D(Q_j). \tag{3.16}$$

In contrast with the first example, the Q_j's are all unbounded self-adjoint operators, whose spectral families $\{F_{j,y}\}$ are given by

$$(F_{j,y} f)(\underline{x}) = \chi_{j,y}(\underline{x}) f(\underline{x}). \tag{3.17}$$

Here $\chi_{j,y}$ is the characteristic function of the region $\{\underline{x} \varepsilon R^n | -\infty < x_j \leq y_j$, other components of $\underline{x}$ unrestricted$\}$ in n-space. As before, we arrive at the interpretation of $|f(\underline{x})|^2$ as the position probability density of the particle in the state f.

The <u>momentum observable</u> is represented by an n-component operator P_j defined as follows.

$$D(P_j) = \{f \varepsilon L^2(R^n) \Big| \int |k_j \tilde{f}(\underline{k})|^2 d^n k < \infty\}$$

and

$$(FP_j f)(\underline{k}) = (h/2\pi) k_j \tilde{f}(\underline{k}), \text{ for all } f \varepsilon D(P_j), \tag{3.18}$$

where $\tilde{f}$ is the Fourier transform of f in $L^2(R^n)$ as defined in (2.26). The P_j's are all unbounded self-adjoint operators. In fact, each P_j is unitarily equivalent to the position operator Q_j. The unitary equivalence is implemented by the Fourier transformation F. This leads naturally to the interpretation of $|\tilde{f}(\underline{k})|^2$ as the momentum probability density of the particle in the state f (Problem 3.3).

It is simple to verify that $S(R^n) \subseteq D(P_j)$. In fact by Proposition 2.4(b), if $f \varepsilon S(R^n)$, then $\tilde{f} \varepsilon S(R^n)$, and since such an $\tilde{f}$ is continuous and rapidly decreasing at infinity, the integral in the definition of $D(P_j)$ converges. Also for $f \varepsilon S(R^n)$, it follows from the definition (3.18) and (2.20)

that

$$(P_j f)(\underline{x}) = (2\pi)^{-n/2} \int e^{i\underline{k}\cdot\underline{x}} (FP_j f)(\underline{k}) d^n k$$

$$= (2\pi)^{-n/2} (h/2\pi) \int e^{i\underline{k}\cdot\underline{x}} k_j \tilde{f}(\underline{k}) d^n k = -i(h/2\pi)\partial f(\underline{x})/\partial x_j . \quad (3.19)$$

Therefore on $S(R^n)$ the momentum operator is $-ih/2\pi$ times the operation of differentiation, which is the customary representation. However it should be emphasized that this restriction of the momentum operator to $S(R^n)$ is only essentially self-adjoint and not self-adjoint. Often (3.18) is said to define the generalized derivative in $L^2(R^n)$.

<u>Example 3.5 : Particle with spin s (s = 0, 1/2, 1, 3/2, ···) in 3-dimensional infinite space.</u>

The appropriate Hilbert space is $L^2(R^3, C^{2s+1})$, i.e. the space of (2s+1)-component functions $f = \{f_m \varepsilon L^2(R^3)$ for each $m = -s, -s+1, \cdots, s-1, s\}$ with inner product

$$(f,g) = \sum_m \int \overline{f_m}(\underline{x}) g_m(\underline{x}) d^3x . \quad (3.20)$$

The position and momentum operators are defined as before, e.g.,

$$D(Q_j) = \{f \varepsilon L^2(R^3, C^{2s+1}) \,\Big|\, \int |x_j f_m(\underline{x})|^2 d^3x < \infty, \text{ for each } m\}$$

and

$$(Q_j f)_m(\underline{x}) = x_j f_m(\underline{x}) . \quad (3.21)$$

Now we introduce a new set of observables called spin, given by a triplet of operators S_1, S_2, S_3. This is done by defining first

$$(S_3 f)_m (\underline{x}) = (h/2\pi)\, m\, f_m(\underline{x}); \; m = -s, -s+1, \ldots, s-1, s$$

$$(S_+ f)_m (\underline{x}) = (h/2\pi) \sqrt{(s+m)(s-m+1)}\, f_{m-1}(\underline{x}) \quad (3.22)$$

and

$$(S_- f)_m (\underline{x}) = (h/2\pi) \sqrt{(s-m)(s+m+1)}\, f_{m+1}(\underline{x}) .$$

It is easy to see that S_3 and $S_\pm$ are bounded linear operators defined everywhere. S_3 is self-adjoint and $S_+^* = S_-$. One then defines bounded self-adjoint operators $S_1 = \frac{1}{2}(S_+ + S_-)$ and $S_2 = -\frac{1}{2}i(S_+ - S_-)$. It can be verified that S_1, S_2, S_3 satisfy the commutation relation $[S_1, S_2] = i(h/2\pi)S_3$ and its cyclic permutations. We also introduce the total spin operator $\underline{S}^2 \equiv S_1^2 + S_2^2 + S_3^2 = S_+S_- - (h/2\pi)S_3 + S_3^2$ which, being a sum of bounded self-adjoint operators, is self-adjoint. Its action in $L^2(R^3, C^{2s+1})$ is as follows (Problem 3.4) :

$$(\underline{S}^2 f)_m(\underline{x}) = s(s+1)(h/2\pi)^2 f_m(\underline{x}).$$

Remark : The introduction of these Hilbert spaces and some of the associated observables may seem a little arbitrary at this stage. Actually there are deeper reasons for the appearance of all the observables introduced so far, viz. the existence of related symmetry groups. In Example 3.4 for instance, one can define space translation symmetry and obtain P_j as the infinitesimal generator of the unitary representation of this symmetry group in $L^2(R^n)$ [P].

So far we have discussed the description of a quantum mechanical system and its relevant observables. This is the analogue of classical kinematics: a particle is described by giving its position and momentum. The next important step is to give the dynamics of the system or equivalently the equation of motion of the system. As already emphasized, here and in the sequel we shall be interested only in the dynamics of pure states. For a description of the dynamics of a general state, the reader is referred to [M, p. 81].

The time-evolution or the dynamics of a conservative

quantum mechanical system is given by a one-parameter unitary group as explained in the introduction to Section 3-1. Let the group be denoted by $\{U_t\}_{t\varepsilon R}$. If the unit vector f represents the state at time t = 0, then the state f_t at time t is given by

$$f_t = U_t f. \tag{3.23}$$

It is clear from the unitarity of U_t that $\|f_t\| = \|f\| = 1$. It is a natural requirement that the expectation value of any observable in a state f at time t be a continuous function of t. This means that $\mathrm{Exp}_{f_t}(A) = (f_t, Af_t)$ is continuous in t. Making a special choice of A, namely a one-dimensional projection F_g, this leads to the conclusion that $|(U_t f,g)|^2$ is continuous in t. Without changing the expectation value or any predictions of the theory, we can choose a phase factor $\xi(t), |\xi(t)| = 1$, such that $(\xi(t)U_t f,g)$ is a continuous function of t and such that $U_t' \equiv \xi(t)U_t$ is still a group [SI]. As mentioned before (Problem 3.1), weak and strong continuity are equivalent for a unitary group. In view of all this we may assume that the time-evolution of a system is given by (3.23) where U_t is a strongly continuous one-parameter unitary group. We shall call equation (3.23) the <u>Schrödinger</u> equation.

Now by Stone's theorem (Proposition 3.1), it follows that there exists a self-adjoint (in general unbounded) operator H given as $Hg = \text{s-lim}\ i(h/2\pi)t^{-1}(U_t - I)g$ as $t \to 0$. This operator plays the same role in quantum mechanics as the Hamiltonian function plays in classical mechanics, viz. the infinitesimal generator of time evolution group, and we shall call this operator the <u>Hamiltonian operator</u>.

Let $f \varepsilon D(H)$. Then $f_t \equiv U_t f \varepsilon D(H)$ by Corollary 3.2(b) and f_t satisfies the differential equation

$$\frac{d}{dt} f_t = -i(h/2\pi)^{-1} H f_t, \tag{3.24}$$

where the derivative is understood as a strong limit. This equation is known in the physics literature as the Schrödinger equation. It has a role parallel to that of Hamilton's equations in classical mechanics. It is a first order differential equation (in a Hilbert space) whose solutions are the trajectories of the (pure) states. In most of this book, by Schrödinger equation we shall mean the integrated form (3.23) and not the differential form (3.24). From (3.24) and (3.23) one sees that, at least formally, the group U_t may be written in terms of its infinitesimal generator as $U_t = \exp(-2\pi i\, Ht/h)$. A precise definition of the exponential function of a self-adjoint operator will be given in Proposition 5.11.

Let f be any eigenvector of H, i.e. $Hf = (h\lambda/2\pi)f$ for some $\lambda \varepsilon R$. Then $U_t f = \exp(-it\lambda)f$ (this follows from the functional calculus developed in Proposition 5.11). $U_t f$ and f differ by a phase factor and hence define the same ray and state. In other words, the expectation value of any (bounded) observable A in the state f_t is the same for all times, because $\mathrm{Exp}_{f_t}(A) = (U_t f, AU_t f) = (f, Af) = \mathrm{Exp}_f(A)$. Such a state is called a <u>stationary state</u>. Conversely, suppose $\mathrm{Exp}_{f_t}(A) = \mathrm{Exp}_f(A)$ for every (bounded) observable. By taking $A = F_g$, where g is any unit vector in H, we have $|(U_t f, g)|^2 = |(f,g)|^2$. In particular, for every vector g such that $(f,g) = 0$, one has $(U_t f, g) = 0$. By the projection theorem, $U_t f$ belongs to the one-dimensional subspace generated by f, i.e. $U_t f = \alpha(t) f$,

where $\alpha(t)$ is a complex-valued continuous one-parameter group. Such a group has a unique representation as an exponential function. Furthermore, since $|\alpha(t)| = 1$, this implies that $\alpha(t) = \exp(-it\lambda)$ for some real λ (Problem 3.6). In the equation $U_t f = \exp(-it\lambda)f$, the right-hand side clearly admits a strong derivative at $t = 0$, so that by Proposition 3.1 $f\varepsilon D(H)$ and $Hf = (h/2\pi)\lambda f$, i.e. f is an eigenvector of H with eigenvalue $(h/2\pi)\lambda$.

We shall call an observable A a <u>constant of motion</u> if $\mathrm{Exp}_{f_t}(F_\lambda) = \mathrm{Exp}_f(F_\lambda)$ for all $f\varepsilon H$ and all real λ and t, where $\{F_\lambda\}$ is the spectral family of A. From the polarization identity (see Problem 2.22) it follows easily that (Problem 3.5)

$$U_t^{-1}F_\lambda U_t = F_\lambda \text{ for all } \lambda \text{ and } t \text{ in } R. \tag{3.25}$$

By Problem 3.11 and Proposition 5.9, this is equivalent to

$$E_\mu F_\lambda = F_\lambda E_\mu \text{ for all } \lambda,\mu\varepsilon R, \tag{3.26}$$

where $\{E_\mu\}$ is the spectral family of the infinitesimal generator H of U_t. When (3.26) is satisfied, one says that the two (possibly unbounded) operators A and H commute. Since H certainly commutes with itself in this sense, the Hamiltonian is a constant of motion and is interpreted as the <u>energy observable</u> of the system.

Let A be any observable (not necessarily a constant of motion) and $\{F_\mu\}$ its spectral family. Then the probability measure $p^A_{I,f_t} \equiv \int_I d(f_t,F_\lambda f_t)$ of the observable A in the evolving state f_t at time t is identical with the probability measure of the evolved observable $A_t \equiv U_t^* A U_t$ at time t in the fixed initial state f. This is so because

$$\int_I d(f_t,F_\lambda f_t) = \int_I d(U_t f,F_\lambda U_t f) = \int_I d(f,U_t^* F_\lambda U_t f)$$

and the family $\{U_t^* F_\lambda U_t\}$ for any fixed t is the spectral family of the self-adjoint operator A_t (Problem 3.5). In the physics literature, these two points of view are distinguished and called the Schrödinger picture (evolving state vector) and the Heisenberg picture (evolving observables) respectively. The equations of evolution (both the differential and the integrated forms) that we have so far given are equations for the state vector and hence appropriate to the Schrödinger picture. One can give equivalent equations of evolution in the Heisenberg picture as follows : One differentiates formally the definition $A_t = U_t^* A U_t$ with respect to t and obtains

$$\frac{dA_t}{dt} = i(h/2\pi)^{-1}(HA_t - A_t H) \equiv i(h/2\pi)^{-1}[H,A_t]. \qquad (3.27)$$

This is called the Heisenberg equation of motion. (This equation is analogous to Hamilton's equation in classical mechanics written in terms of Poisson brackets, i.e. $dA/dt = -\{H,A\}$, where A is any classical observable and H is the Hamilton function.) When both A and H are bounded, the equation makes sense on any vector in $\mathcal{H}$. The general case when A and H are unbounded self-adjoint operators is more complicated, and it is precisely for this reason that we shall not use the differential version of either the Schrödinger or the Heisenberg equation.

We still have not reached a stage where we can actually compute the motion of the particle given the initial state f at time t = 0. What we have done is similar to writing down Newton's equation $\underline{F} = m\ddot{\underline{q}}$, but we cannot start computing

until we know the force $\underline{F}$. In fact, we can distinguish between various classical theories by what we take for $\underline{F}$ or equivalently for the Hamilton function $H(\underline{p},\underline{q})$. Likewise, we can have various quantum mechanical theories by making appropriate choices for H. For every physical system, the choice of H is dictated by the underlying dynamical symmetry group and by the corresponding classical Hamilton function if one has any. For example, in non-relativistic physics the principle of Galilean relativity leads to the invariance of the theory under the Galilean symmetry group and this in turn restricts the Hamilton function for a single particle in non-relativistic classical mechanics to be of the form $H(\underline{p},\underline{q}) = \underline{p}^2/2m + V(\underline{q})$, where V is called the potential function and $\underline{p}^2/2m$ is the kinetic energy. Then various non-relativistic theories will be distinguished by the choice of the potential function V. For a more elaborate discussion of these points, the reader is referred to [P]. In quantum mechanics, one has the task of making H a self-adjoint operator after one has obtained a form for it from physical considerations. A study of this question is deferred until Chapter 8, and in this section we shall be content with giving a few simple examples.

Example 3.6 : Free non-relativistic spinless particle in R^n.

Classically the Hamilton function is given by $H = \underline{p}^2/2m$, where m is identified with the inertial mass of the particle. Reminding ourselves that the appropriate Hilbert space for the description of such a quantum mechanical system is $L^2(R^n)$, in which the momentum operators P_j are defined

by (3.18), we write the Hamiltonian operator for a free particle as $K_o = (2m)^{-1} \sum_{j=1}^{n} P_j^2$, defined as follows :

$$D(K_o) = \{f \varepsilon L^2(R^n) \mid \int |\underline{k}^2 \tilde{f}(\underline{k})|^2 d^n k < \infty\} \tag{3.28}$$

and $$(FK_o f)(\underline{k}) = (2m)^{-1}(h/2\pi)^2 \underline{k}^2 \tilde{f}(\underline{k}), \text{ for } f \varepsilon D(K_o). \tag{3.29}$$

By Proposition 2.16, K_o is a self-adjoint operator. Furthermore, if $f \varepsilon S(R^n)$, then it is easy to show that

$$(K_o f)(\underline{x}) = -(2m)^{-1}(h/2\pi)^2 (\Delta f)(\underline{x}), \tag{3.30}$$

where Δ is the Laplacian $\sum_{j=1}^{n} \partial^2/\partial x_j^2$. Thus for $f \varepsilon S(R^n)$ one can write down the free Schrödinger equation in differential form as $df_t/dt = -(2m)^{-1}(h/2\pi)^2 \Delta f_t$. In the next section we shall return to this example and establish various properties of the above operator K_o.

Example 3.7 : Spinning electron in a constant magnetic field.

It is experimentally observed and also theoretically predicted that an electron carries with it a magnetic (dipole) moment given by $\underline{\mu} = g\mu_B \underline{S}$, where $\mu_B = eh(4\pi mc)^{-1}$ is the Bohr magneton. g is the gyromagnetic ratio of the electron (very close to 2) and $\underline{S}$ is the spin-triplet observable, with $s = \frac{1}{2}$. In this case, again by analogy with the classical theory, the Hamiltonian operator is formally given by the energy of interaction between the moment associated with the electron and the magnetic field, i.e. $H = -\underline{\mu}.\underline{B}$, where $\underline{B}$ is the magnetic field intensity vector. The relevant Hilbert space being $L^2(R^3, C^2)$, we conclude that $H = -g\mu_B|\underline{B}|S_3$, where we have chosen the third direction in R^3 to be the one parallel to the field $\underline{B}$. Since S_3 is a bounded self-adjoint operator in

$L^2(R^3, C^2)$, so is H (see Example 3.5).

Example 3.8 : Spinless relativistic free particle in R^n.

We know that the energy of a classical relativistic free particle is given by $K_o^R = (m^2c^4 + \underline{p}^2c^2)^{\frac{1}{2}}$, where $\underline{p}$ is its momentum, c is the speed of light and m is the rest mass. So the Hamiltonian operator is defined as :

$$D(K_o^R) = \{f\varepsilon L^2(R^n) \mid \int \underline{k}^2|\tilde{f}(\underline{k})|^2 d^n k < \infty\} \tag{3.31}$$

and for $f\varepsilon D(K_o^R)$, $(FK_o^R f)(\underline{k}) = [m^2c^4 + (h/2\pi)^2\underline{k}^2c^2]^{\frac{1}{2}}\tilde{f}(\underline{k})$.

As before, Proposition 2.16 shows that this is a self-adjoint operator.

3-3 FREE NON-RELATIVISTIC DYNAMICS

In this section we study in detail various properties of the operator K_o, the Hamiltonian of a spinless non-relativistic free particle, introduced in the last section. We also obtain a certain convenient description of the free time-evolution operator U_t associated with K_o which will be very useful in scattering theory. We end the section with some results on asymptotic position probability measures for $t\to\pm\infty$.

For convenience of presentation, from now on we shall set $h/2\pi = 2m = 1$, keeping in mind that, whenever physical quantities are computed and a comparison with experimental results is attempted, $h/2\pi$ and m have to be reintroduced. This simplifies various expressions, e.g. for $f\varepsilon D(K_o)$,

$(FK_o f)(\underline{k}) = \underline{k}^2 \tilde{f}(\underline{k})$ instead of (3.29). We have seen that K_o is a self-adjoint operator and that its restriction to $S \equiv S(R^n)$ is $-\Delta$. Now we prove

PROPOSITION 3.9 : K_o restricted to $S(R^n)$ is essentially self-adjoint.

Proof : We recall from Corollary 2.15 that a symmetric operator A is essentially self-adjoint if and only if the ranges of the operators $(A \pm i)$ are dense in H. $K_{o|S}$ *) is symmetric since it is the restriction of the self-adjoint operator K_o to a dense subset S of its domain $D(K_o)$. Since for $g \varepsilon S$ $(F(K_o \pm i)g)(\underline{k}) = (\underline{k}^2 \pm i)\tilde{g}(\underline{k})$ and multiplication by $(\underline{k}^2 \pm i)$ maps S onto itself in a one-to-one fashion, it follows that the operators $(K_{o|S} \pm i)$ map S onto itself, once we remember from Proposition 2.4 (b) that the Fourier transformation leaves S invariant. Therefore, the ranges of $(K_{o|S} \pm i)$ are S and hence dense. This completes the proof. #

Remark : It is also true that K_o restricted to $C_o^\infty(R^n)$ is essentially self-adjoint. For this it suffices to show that $K_{o|S} \subseteq \overline{K_{o|C_o^\infty}}$, because we know that $K_{o|C_o^\infty} \subseteq K_{o|S}$ and therefore $\overline{K_{o|C_o^\infty}} \subseteq \overline{K_{o|S}} = K_o$. To this end we need to construct for every $g \varepsilon S(R^n)$ a sequence $g_n \varepsilon C_o^\infty(R^n)$ such that s-lim $g_n = g$ and s-lim $K_o g_n = K_o g$, which can be shown to be possible (Problem 3.7).

The self-adjoint operator K_o is not a differential operator in the usual sense because a function $f(\underline{x})$ in $D(K_o)$

*) $A|_D$ denotes the restriction of the operator A to a subset $D \subseteq D(A)$.

need not be differentiable. Nevertheless, for $n = 3$ the functions in $D(K_0)$ have a certain regularity property as proven in

PROPOSITION 3.10 : Let $n = 3$. Then every $f \varepsilon D(K_0)$ is (equivalent to) a bounded, uniformly continuous function of $\underline{x}$.

Proof : Let $\alpha > 0$. Then

$$\int_{R^3} (\underline{k}^2 + \alpha^2)^{-2} \, d^3k = 4\pi \int_0^\infty (k^2 + \alpha^2)^{-2} \, k^2 dk = \pi^2/\alpha.$$

By applying the Schwarz inequality in $L^2(R^3)$ we obtain that

$$[\int |\tilde{f}(\underline{k})| \, d^3k]^2 = [\int |(\underline{k}^2 + \alpha^2)\tilde{f}(\underline{k})| \, (\underline{k}^2 + \alpha^2)^{-1} \, d^3k]^2$$

$$\leq \frac{\pi^2}{\alpha} \int |(\underline{k}^2 + \alpha^2)\tilde{f}(\underline{k})|^2 \, d^3k = \frac{\pi^2}{\alpha} \, \|(K_0 + \alpha^2)f\|^2 < \infty.$$

Therefore $\tilde{f} \varepsilon L^1(R^3)$. It now follows from (2.20) that $f(\underline{x})$ is bounded :

$$|f(\underline{x})| \leq (2\pi)^{-3/2} \int |\tilde{f}(\underline{k})| \, d^3k \leq c \, \alpha^{-1/2} \, \|(K_0 + \alpha^2)f\|$$

$$\leq c \, (\alpha^{-1/2} \, \|K_0 f\| + \alpha^{3/2} \, \|f\| \,). \tag{3.32}$$

Similarly one infers the continuity of $f(\underline{x})$ from (2.20) and the Lebesgue dominated convergence theorem (see also Problem 3.10). #

Remark : The above result is a special case of the Sobolev inequality [SO] and depends essentially on the dimension 3 of the space.

We now study properties of the one-parameter unitary group corresponding to K_0. These will be frequently used in later chapters. We define for $t \varepsilon R$ and $f \varepsilon L^2(R^n)$

$$(FU_t f)(\underline{k}) = \exp(-i\underline{k}^2 t)\tilde{f}(\underline{k}) \tag{3.33}$$

and first prove

PROPOSITION 3.11 : $\{U_t\}$ defined by (3.33) forms a continuous one-parameter unitary group in $L^2(R^n)$, and its infinitesimal generator is K_o.

Proof : (i) The group property of $\{U_t\}$ is an immediate consequence of the definition (3.33). Its continuity follows provided that we can show that U_t is weakly continuous at $t = 0$ (see Problem 3.1). This is done as follows:

$$(f,(U_t-I)g) = \int \bar{\tilde{f}}(\underline{k})[\exp(-i\underline{k}^2t)-1]\tilde{g}(\underline{k})d^nk.$$

The integrand converges pointwise to zero as $t\to 0$ and is uniformly (with respect to t) majorized by $2|\tilde{f}(\underline{k})\tilde{g}(\underline{k})|$, which is integrable since f and g are in $L^2(R^n)$. Then by the Lebesgue dominated convergence theorem, $(f,(U_t-I)g)$ converges to zero as $t\to 0$.

(ii) (3.33) implies that $\|U_tf\|^2 = \|\tilde{f}\|^2 = \|f\|^2$ and $(f,U_tg) = (U_{-t}f,g)$. The first of these two identities shows that U_t is defined everywhere, and the second one that $U_t^* = U_{-t}$. Hence $U_t^*U_t = U_{-t}U_t = I$ and $U_tU_t^* = I$, i.e. U_t is unitary.

(iii) One has for $\alpha\varepsilon R$

$$|it^{-1}[\exp(-it\alpha)-1] - \alpha| = |\int_0^\alpha[\exp(-its)-1]ds| \leq 2\alpha. \quad (3.34)$$

Now let $f\varepsilon D(K_o)$. Then $\|[it^{-1}(U_t-I) - K_o]f\|^2 =$

$$\int|\tilde{f}(\underline{k})|^2|it^{-1}[\exp(-it\underline{k}^2)-1] - \underline{k}^2|^2\, d^nk. \quad (3.35)$$

The integrand in (3.35) converges pointwise to zero, and by (3.34) the integrand is majorized uniformly in t by $4|\underline{k}^2\tilde{f}(\underline{k})|^2$, which is integrable. Hence the Lebesgue dominated convergence

theorem allows us to conclude that

$$\operatorname*{s-lim}_{t\to 0} [it^{-1}(U_t-I)-K_0]f = \theta \text{ for all } f\varepsilon D(K_0).$$

Therefore the infinitesimal generator of U_t is equal to K_0 on $D(K_0)$. Since K_0 is self-adjoint, the infinitesimal generator of U_t must be K_0. #

U_t defined by (3.33) gives the evolution operator for a free non-relativistic particle. Passing to the $\underline{x}$-representation we write

$$(U_t f)(\underline{x}) = \ell.i.m.(2\pi)^{-n/2}\int e^{i\underline{k}\cdot\underline{x}} e^{-ik^2 t}\tilde{f}(\underline{k})\, d^n k. \qquad (3.36)$$

The following lemma and its corollary play a crucial role in scattering theory.

<u>LEMMA 3.12</u> : Let $f\varepsilon L^1(R^n)\cap L^2(R^n)$ and $t \neq 0$. Then

$$(U_t f)(\underline{x}) = (4\pi it)^{-n/2}\int \exp(i|\underline{x}-\underline{y}|^2/4t) f(\underline{y})\, d^n y, \qquad (3.37)$$

where the branch of the square-root is chosen so that

$$(4\pi it)^{-n/2} = |4\pi t|^{-n/2} \cdot \begin{cases} \exp(-in\pi/4) & \text{if } t > 0 \\ \exp(in\pi/4) & \text{if } t < 0. \end{cases}$$

<u>Proof</u> : (i) We shall prove the lemma for $n = 1$, since the extension to the general case is straightforward. The right-hand side of the relation (3.36) is an ordinary integral if $f\varepsilon S(R)$. In particular, for $f_a(x) \equiv \exp[-(x-a)^2]$, an elementary calculation shows that

$$\begin{aligned}(U_t f_a)(x) &= (2\pi)^{-\frac{1}{2}}\int e^{ikx}\, e^{-ik^2 t}\tilde{f}_a(k)\, dk \\ &= (4\pi)^{-\frac{1}{2}}\int e^{ikx}\, e^{-ik^2 t} e^{-k^2/4}\, e^{-ika}\, dk \\ &= (1 + 4it)^{-\frac{1}{2}} \exp\{-(x-a)^2/(1 + 4it)\}, \qquad (3.38)\end{aligned}$$

where for complex α we have chosen the branch of the square root so that $\mathrm{Re}\sqrt{\alpha} > 0$ and used the fact that the Fourier transform of $\exp(-\alpha x^2/2)$ is $\alpha^{-\frac{1}{2}}\exp(-k^2/2\alpha)$ (see Problem 2.10). On the other hand,

$$(4\pi it)^{-\frac{1}{2}}\int\exp(i|x-y|^2/4t)f_a(y)dy = (2it)^{-\frac{1}{2}}\exp(i|x-a|^2/4t)\cdot$$

$$(2\pi)^{-\frac{1}{2}}\int\exp[-i(y-a)(x-a)/2t]\exp[-(y-a)^2(1-i/4t)]dy$$

$$= (1+4it)^{-\frac{1}{2}}\exp[-(x-a)^2/(1+4it)]. \tag{3.39}$$

Comparing (3.38) and (3.39) we arrive at (3.37) for each f_a and hence for the set $\mathcal{D}$ consisting of finite linear combinations of such functions, i.e.

$$(U_t f)(x) = (4\pi it)^{-\frac{1}{2}}\int\exp(i|x-y|^2/4t)f(y)dy \tag{3.40}$$

for all $f\varepsilon\mathcal{D}$.

(ii) Next we claim that $\mathcal{D}$ is dense in $L^2(R)$. To see this let g be any vector orthogonal to f_a for all a. Then by (2.23) $\int\bar{\tilde{g}}(k)\exp(-ika-k^2/4)dk = 0$. This means that the Fourier transform of the function $\bar{\tilde{g}}(k)\exp(-k^2/4)$ at a equals zero. By the unitarity of F, $\tilde{g} = 0$ a.e. or $g = \theta$. Hence $\mathcal{D}$ is dense by the denseness criterion on page 28.

(iii) We know from Proposition 3.11 that $\|U_t f\| = \|f\|$. Therefore, the relation (3.40) can be extended to the whole of $L^2(R)$ and written

$$(U_t f)(x) = \ell.\mathrm{i.m.}(4\pi it)^{-\frac{1}{2}}\int\exp[i(x-y)^2/4t]f(y)dy, \tag{3.41}$$

just as was the case with the Fourier transformation. In particular, if $f\varepsilon L^1(R)\cap L^2(R)$, then the right-hand side makes sense as an ordinary integral and (3.37) is valid. #

COROLLARY 3.13 : Let $f \varepsilon L^1(R^n) \cap L^2(R^n)$, $t \neq 0$. Then $U_t f$ is a bounded function of $\underline{x}$ and

$$\sup_{\underline{x} \varepsilon R^n} |(U_t f)(\underline{x})| \leq |4\pi t|^{-n/2} \|f\|_1 \tag{3.42}$$

The proof follows immediately from (3.37).

Remark 3.14 : We can rewrite (3.41) in n dimensions as

$$(U_t f)(\underline{x}) = \ell.i.m. \int K(\underline{x}-\underline{y};t)\ f(\underline{y})\ d^n y, \tag{3.43}$$

where $$K(\underline{x}-\underline{y};t) = (4\pi i t)^{-n/2} \exp[i(\underline{x}-\underline{y})^2/4t]. \tag{3.44}$$

The integral kernel $K(\underline{x}-\underline{y};t)$ is called the free propagator.

Remark 3.15 : An interesting consequence of the inequality (3.42) is the following. Let Δ be a measurable set in R^n with Lebesgue measure $|\Delta| < \infty$ and F_Δ the projection operator in $L^2(R^n)$ associated with the set Δ by (2.39). Then the probability of finding the freely evolving particle at time t in the set Δ tends to zero as $t \to \pm\infty$ or equivalently,

$$\|F_\Delta U_t f\|^2 \to 0 \text{ as } t \to \pm\infty \text{ for all } f \varepsilon L^2(R^n). \tag{3.45}$$

For a proof of this, one notes that by (3.42) one has for all $f \varepsilon S(R^n)$

$$\|F_\Delta U_t f\|^2 = \int_\Delta |(U_t f)(\underline{x})|^2\ d^n x \leq |4\pi t|^{-n} |\Delta|\ \|f\|_1^2,$$

which tends to zero as $t \to \pm\infty$. Since $S(R^n)$ is dense in $L^2(R^n)$ and since $\|F_\Delta U_t\| \leq 1$, we arrive at (3.45) by using Proposition 2.17.

For further discussion, it is useful to factorize U_t into a product of two simpler operators as defined in the following lemma.

LEMMA 3.16 : Suppose $t \neq 0$. Define two linear operators C_t and Q_t in $L^2(R^n)$ by

$$\begin{aligned}(C_t f)(\underline{x}) &= (2it)^{-n/2}\exp(i\underline{x}^2/4t)\tilde{f}(\underline{x}/2t)\\ (Q_t f)(\underline{x}) &= \exp(i\underline{x}^2/4t)f(\underline{x})\end{aligned} \tag{3.46}$$

Then C_t and Q_t are unitary operators and

$$U_t = C_t Q_t \ . \tag{3.47}$$

Proof : The unitarity of Q_t is obvious and that of C_t follows from the unitarity of the Fourier transformation. Since U_t and $C_t Q_t$ are both unitary operators, we need to establish their equality on a dense domain and then extend the result to the whole of $L^2(R^n)$ by Lemma 2.27. Let $f \varepsilon S(R^n)$. Then by (3.37) we write

$$(U_t f)(\underline{x}) = (2it)^{-n/2}(2\pi)^{-n/2}\int \exp(i|\underline{x}-\underline{y}|^2/4t)f(\underline{y})d^n y$$

$$= (2it)^{-n/2}\exp(i\underline{x}^2/4t)(2\pi)^{-n/2}\int\exp(-i\underline{y}\cdot\underline{x}/2t)\exp(i\underline{y}^2/4t)f(y)d^n y$$

$$= (2it)^{-n/2}\exp(i\underline{x}^2/4t)(2\pi)^{-n/2}\int\exp(-i\underline{y}\cdot\underline{x}/2t)(Q_t f)(\underline{y})d^n y$$

$$= (2it)^{-n/2}\exp(i\underline{x}^2/4t)\ (FQ_t f)(\underline{x}/2t) = (C_t Q_t f)(\underline{x}). \ \#$$

The next proposition establishes the asymptotic behaviour of U_t for $t \to \pm\infty$.

PROPOSITION 3.17 : Let $f \varepsilon L^2(R^n)$. Then

$$\lim_{t\to\pm\infty} \|U_t f - C_t f\| = 0. \tag{3.48}$$

Proof : Using Lemma 3.16 and the unitarity of C_t, we have

$$\|U_t f - C_t f\|^2 = \|C_t Q_t f - C_t f\|^2 = \|Q_t f - f\|^2$$

$$= \int|\exp(i\underline{x}^2/4t) - 1|^2|f(\underline{x})|^2\ d^n x.$$

Since the integrand is bounded by the integrable function $4|f(\underline{x})|^2$ and converges pointwise to zero as $t\to\pm\infty$, an application of the dominated convergence theorem leads to the desired result. #

The Proposition 3.17 leads naturally to the following observation. Let Δ be a measurable subset of R^n and f be a vector in $L^2(R^n)$. Then

$$\left|\int_\Delta |(U_t f)(\underline{x})|^2 d^n x - \int_\Delta |(C_t f)(\underline{x})|^2 d^n x\right| = \left| \|F_\Delta U_t f\|^2 - \|F_\Delta C_t f\|^2\right|$$

$$= (\|F_\Delta U_t f\| + \|F_\Delta C_t f\|)\left| \|F_\Delta U_t f\| - \|F_\Delta C_t f\|\right|. \qquad (3.49)$$

By applying the inequality (2.88) and observing that $\|F_\Delta\| \leq 1$, we see that the last member of (3.49) is majorized by $2\|f\|\,\|U_t f - C_t f\|$, which by virtue of Proposition 3.17 goes to zero as $t\to\pm\infty$. This means that given an initial state $f\varepsilon L^2(R^n)$, $\|f\| = 1$, the position probability measure over any measurable subset $\Delta \subseteq R^n$ for the freely evolving state $U_t f$ can be asymptotically replaced by that of the state $C_t f$, i.e.

$$\lim_{t\to\pm\infty} \int_\Delta |(U_t f)(\underline{x})|^2 d^n x = \lim_{t\to\pm\infty} \int_\Delta |(C_t f)(\underline{x})|^2 d^n x$$

in the sense that if the limit on one side exists, so does the other and they are equal.

Now

$$|(C_t f)(\underline{x})|^2 = |2t|^{-n} |\tilde{f}(\underline{x}/2t)|^2, \qquad (3.50)$$

so that for large positive or negative times the position probability density of the freely evolving state f can be replaced by $|2t|^{-n}|\tilde{f}(\underline{x}/2t)|^2$, which is simply the probability that it has momentum $\underline{x}/2t$, the correct classical momentum to get from the origin to the point $\underline{x}$ in time t.

As an example, we compute the asymptotic probability $P^{\pm}_{free}(f,C)$ that the particle with initial state f, evolving freely, will be found as $t\to\pm\infty$ in a cone C with apex at the origin. From the definition it follows that

$$P^{\pm}_{free}(f,C) = \lim_{t\to\pm\infty} \int_C |(U_t f)(\underline{x})|^2 d^n x$$

$$= \lim_{t\to\pm\infty} \int_C |2t|^{-n} |\tilde{f}(\underline{x}/2t)|^2 d^n x = \int_{\pm C} |\tilde{f}(\underline{k})|^2 d^n k. \qquad (3.51)$$

The last step follows by making the change of variable $\underline{k} = \underline{x}/2t$ in the integral over C. This maps C onto itself or its reflection through the origin depending on whether $t > 0$ or $t < 0$. This explains the appearance of "$\pm C$" in the final result. This expression conforms to the intuition that for large positive (or negative) times the probability that the particle will be in C is the same as the probability that its momentum lies in the cone +C (respectively -C). A generalization of (3.51) for interacting particles will be given in Sections 7-3 and 15-3.

3-4 NOTES AND SUPPLEMENTARY MATERIAL

A. Proof of Theorem 3.1 :

(i) Define $R_{+i}f = i\int_0^\infty e^{-s} U_s f\, ds$

and $R_{-i}f = -i\int_{-\infty}^0 e^{s} U_s f\, ds$, for $f\varepsilon H$. (3.52)

At this point we shall not dwell on the definition of these integrals, except to say that they can be defined as strong limits of Riemann sums of vectors, similar to the ordinary Riemann integrals. More will be said on this in Section 4-4. From the definition it is clear that $\|R_{\pm i}f\| \le \|f\|$ for all

$f\varepsilon H$, or in other words, $R_{\pm i}$ are bounded linear operators defined everywhere.

(ii) Now we show that the strong derivative of U_t at $t = 0$ exists on the ranges of $R_{\pm i}$. Let f be any vector in H. Then

$$i\tau^{-1}(U_\tau - I)R_{+i}f = -\tau^{-1}\int_0^\infty e^{-s}U_{s+\tau}f\,ds + \tau^{-1}\int_0^\infty e^{-s}U_s f\,ds$$

$$= -\tau^{-1}(e^\tau - 1)\int_\tau^\infty e^{-\sigma}U_\sigma f\,d\sigma + \tau^{-1}\int_0^\tau e^{-s}U_s f\,ds$$

$$= \tau^{-1}(e^\tau - 1)\,\{iR_{+i}f + \int_0^\tau e^{-\sigma}U_\sigma f\,d\sigma\} + \tau^{-1}\int_0^\tau e^{-s}U_s f\,ds.$$

By continuity of $e^{-s}U_s f$, the second term tends to f as $\tau \to 0$. Similarly, the first term tends to $iR_{+i}f$. This leads to the conclusion that the strong derivative of U_t exists on $R_{+i}H$. A similar conclusion follows for $R_{-i}H$, and we have

$$AR_{\pm i}f = \pm iR_{\pm i}f + f \text{ for all } f\varepsilon H. \tag{3.53}$$

(iii) Next we prove that $R_{+i}H$ is dense in H. Suppose g is orthogonal to $R_{+i}H$, i.e. $(g,R_{+i}f) = 0$ for all $f\varepsilon H$. Now, since $U_tU_s = U_sU_t = U_{t+s}$ it follows from the definition (3.52) that U_t commutes with R_{+i} and hence that U_t leaves $R_{+i}H$ invariant. Therefore

$$(g,U_tR_{+i}f) = 0 \text{ for all } f\varepsilon H. \tag{3.54}$$

Then using (3.52) and (3.54), one gets

$$\int_0^\infty e^{-s}(g,U_{s+t}f)ds = e^t\int_t^\infty e^{-\sigma}(g,U_\sigma f)d\sigma = 0,$$

or

$$\int_t^\infty e^{-\sigma}(g,U_\sigma f)d\sigma = 0\,. \tag{3.55}$$

Since (3.55) is true for all t, a differentiation with respect to t along with the observation that the integrand is a continuous function leads to the conclusion that $(g,U_tf) = 0$

for all t. In particular $(g,f) = 0$. Since f is an arbitrary vector in $\mathcal{H}$, it follows that $g = \theta$, so that by the statement following the projection theorem on page 28, $R_i\mathcal{H}$ is dense in $\mathcal{H}$. A similar conclusion follows for $R_{-i}\mathcal{H}$.

So far we have shown that $R_{\pm i}\mathcal{H} \subseteq D(A)$ and that $R_{\pm i}\mathcal{H}$ are dense in $\mathcal{H}$, so that A is a densely defined linear operator.

(iv) Here we prove that A is symmetric. Let $f,g\varepsilon D(A)$. Then $(Af,g) = \lim_{t\to 0} (it^{-1}(U_t-I)f,g) = \lim (f,-it^{-1}(U_{-t}-I)g) = (f,Ag)$. Now for all $f\varepsilon D(A)$, $\|(A\pm i)f\|^2 = \|Af\|^2 + \|f\|^2$ by (2.48). Therefore, $(A\pm iI)f = \theta$ implies $\|f\| = 0$, hence $f = \theta$. Thus $(A\pm i)$ are also invertible.

(v) Finally we claim that the operators $(A\pm i)$ map $D(A)$ onto $\mathcal{H}$. The equation (3.53) can be rewritten as

$$(A\mp i)R_{\pm i}f = f, \text{ for all } f\varepsilon\mathcal{H}. \tag{3.56}$$

It follows that $(A\mp i)$ map $R_{\pm i}\mathcal{H}$ onto $\mathcal{H}$. A fortiori they map $D(A)$ onto $\mathcal{H}$, since $R_{\pm i}\mathcal{H} \subseteq D(A)$. It now follows from Proposition 2.14 that A is self-adjoint, which completes the proof. #

We may add that (3.56) has the following interesting consequences (obtained upon multiplication by $(A\mp i)^{-1}$) :

$$R_{\pm i} = (A\mp i)^{-1} \text{ and hence } R_{\pm i}\mathcal{H} = D(A). \tag{3.57}$$

In fact, similar statements can be made for any complex number z ($\operatorname{Im} z \neq 0$) in place of $\pm i$, viz. $(A-z)^{-1} \varepsilon \mathcal{B}(\mathcal{H})$ and

$$(A-z)^{-1} = \begin{cases} i\int_0^\infty e^{izs}U_s ds; & \operatorname{Im} z > 0 \\ -i\int_{-\infty}^0 e^{izs}U_s ds; & \operatorname{Im} z < 0. \end{cases} \tag{3.58}$$

The operator $(A-z)^{-1}$ is called the <u>resolvent</u> of the self-

adjoint operator A and denoted by $R_z(A)$ or simply be R_z when only one operator A is involved. We shall return to resolvents and their properties in Chapter 5. The verification of the relation (3.58) is left as an exercise (Problem 3.8).

B. We end this section with the following remarks with reference to Corollary 3.13. For this purpose, we define L^p-spaces ($p \geq 1$) in a manner similar to that of Section 2-2. They consist of all Lebesgue measurable complex-valued functions on R^n which satisfy the following condition, viz.

$$\int_{R^n} |f(\underline{x})|^p d^n x < \infty . \tag{3.59}$$

It is well-known that the set of all such functions forms a vector space under the usual rules of addition and multiplication by complex scalars. As in the case of L^2, one says that two functions are equivalent if they differ only on a set of Lebesgue measure zero. Then $L^p(R^n)$ is defined to be the space of equivalence classes of such functions, satisfying (3.59). It can be shown that $L^p(R^n)$ is complete with respect to the norm defined as follows :

$$\|f\|_p = (\int |f(\underline{x})|^p d^n x)^{1/p}. \tag{3.60}$$

One important property of L^p-spaces is the Hölder inequality. It states that if $p^{-1} + q^{-1} = 1$ and if $f \varepsilon L^p(R^n)$ and $g \varepsilon L^q(R^n)$, then the product function $\bar{f} \cdot g$ (defined as $(\bar{f} \cdot g)(\underline{x}) = \overline{f(\underline{x})} g(\underline{x})$) belongs to $L^1(R^n)$ and furthermore,

$$|\int \bar{f}(\underline{x}) g(\underline{x}) d^n x| \leq \|f\|_p \|g\|_q . \tag{3.61}$$

It is clear that the Schwarz inequality for the Hilbert space $L^2(R^n)$ appears as a special case of (3.61) when $p = q = 2$.

One has similarly a generalisation of (3.42). Let $1 \leq p < 2$, $p^{-1} + q^{-1} = 1$ and $f \varepsilon L^p(R^n) \cap L^2(R^n)$. Then it can be shown using (3.61) and Hausdorff-Young inequality, that $U_t f \varepsilon L^q(R^n) \cap L^2(R^n)$ and

$$\|U_t f\|_q \leq c\ |t|^{-n(p^{-1}-\frac{1}{2})} \|f\|_p. \tag{3.62}$$

For a proof of (3.62), the reader may consult [RS II, Section IX.7].

The operators C_t and Q_t, used to prove (3.51), were introduced by Dollard [3].

PROBLEMS

3.1 : Show that for one-parameter unitary groups $\{U_t\}$, strong continuity at arbitrary t is equivalent to strong continuity at t = o and that strong continuity is equivalent to weak continuity. (Hint : Use Proposition 2.1.)

3.2 : Verify that the operators defined by the relation (3.13) satisfy the properties (3.7)-(3.10).

3.3 : Starting from the definition (3.18), construct the spectral family for the n-component momentum operator $\{P_j\}$ and show that $|\tilde{f}(\underline{k})|^2$ is the momentum probability density.

3.4 : Verify from the definition (3.22) (with $h = 2\pi$) that
(a) each S_j is self-adjoint and $S_+^* = S_-$,
(b) $[S_1, S_2] = iS_3$ and its cyclic permutations,
(c) $(\underline{S}^2 f)_m(\underline{x}) = s(s+1) f_m(\underline{x})$ and that $\underline{S}^2$ is a bounded self-adjoint operator.

3.5 : Let A be an observable and $\{F_\lambda\}$ its spectral family. (a) Show that under suitable domain conditions the family $\{U_t^* F_\lambda U_t\}$, for each fixed t, is the spectral family of the self-adjoint operator $A_t \equiv U_t^* A U_t$. (b) If furthermore, $\mathrm{Exp}_{f_t}(F_\lambda) = \mathrm{Exp}_f(F_\lambda)$ for all $f \varepsilon H$ and $\lambda, t \varepsilon R$, then $U_t^* F_\lambda U_t = F_\lambda$.

3.6 : Let $\alpha(t)$ be a complex-valued continuous one-parameter group. Prove that $\alpha(t)$ admits a unique representation as

$\alpha(t) = \exp(\beta t)$, where β is a complex number. (Hint : Show that continuity implies differentiability by using the identity $\int_t^{t+\tau}\alpha(s)ds = \alpha(t)\int_0^{\tau}\alpha(s)ds$.)

3.7 : Let g be a function in $\mathcal{S}(R^n)$. Construct a sequence of functions g_n in $C_0^\infty(R^n)$ such that s-lim $g_n = g$ and s-lim $K_0 g_n = K_0 g$. (Hint : Write $g_n(\underline{x}) = \phi(\underline{x}/n)g(\underline{x})$, where ϕ is a C_0^∞-function such that $0 \leq \phi(\underline{x}) \leq 1$ and $\phi(\underline{x}) = 1$ for $|\underline{x}| \leq 1$, and use the Lebesgue dominated convergence theorem.)

3.8† : Let U_t,A be as in Proposition 3.1. Show that for any complex number z (Im $z \neq 0$), the operator $(A-z)^{-1}$ is bounded and defined everywhere and verifies (3.58).

3.9 : Show that for $z \notin [o,\infty)$, $(K_0-z)^{-1}$ is a bounded operator with domain $\mathcal{H}$. Verify that for any $f,g\varepsilon\mathcal{H}$ and Im $z > 0$, $(f,(K_0-z)^{-1}g) = i\int_0^\infty dt\, \exp(izt)(f,\exp(-iK_0 t)g)$.

3.10 : Prove the uniform continuity in Proposition 3.10. Hint : Verify and use the inequality

$$|e^{i\alpha}-e^{i\beta}| \leq 2^{1-\nu}|\alpha-\beta|^\nu \text{ for } 0 \leq \nu \leq 1,\ \alpha,\beta\varepsilon R. \qquad (3.63)$$

3.11 : Let U_t,A and D(A) be as in Proposition 3.1 and $B \varepsilon \mathcal{B}(\mathcal{H})$. Assume that $BU_t = U_t B$ for all t. Prove that B leaves D(A) invariant and that, for $f \varepsilon D(A)$, BAf = ABf, i.e. BA $\subseteq$ AB. If furthermore $B^{-1} \varepsilon \mathcal{B}(\mathcal{H})$, then BA = AB. (See also page 187).