X.12 Time-dependent Hamiltonians

In this section we prove two existence theorems for the time-dependent Schrödinger equation

$$\frac{d\varphi(t)}{dt} = -iH(t)\varphi(t) \tag{X.127}$$

The investigation of time-dependent problems is important because one sometimes wants to calculate the change in a quantum system in a variety of situations, for example, when an external potential is turned on and then switched off after a short time or when a periodic potential is turned on. We first introduce the analogue of unitary one-parameter groups.

Definition A two-parameter family of unitary operators $U(s, t)$, $s, t \in \mathbb{R}$ which satisfies:

(a) $U(r, s)U(s, t) = U(r, t)$
(b) $U(t, t) = I$
(c) $U(s, t)$ is jointly strongly continuous in s and t

is called a **unitary propagator**.

Theorem X.69 (the Dyson expansion) Let $t \to H(t)$ be a strongly continuous map of $\mathbb{R}$ into the *bounded* self-adjoint operators on a Hilbert space $\mathscr{H}$. Then there is a unitary propagator on $\mathscr{H}$ so that, for all $\psi \in \mathscr{H}$,

$$\varphi_s(t) = U(t, s)\psi$$

satisfies

$$\frac{d}{dt}\varphi_s(t) = -iH(t)\varphi_s(t), \qquad \varphi_s(s) = \psi \tag{X.128}$$

Proof We define

$$U(t, s)\varphi = 1 + \sum_{n=1}^{\infty} (-i)^n \int_s^t \int_s^{t_1} \cdots \int_s^{t_{n-1}} H(t_1) \cdots H(t_n)\varphi \, dt_n \cdots dt_1 \tag{X.129}$$

By the uniform boundedness principle, $H(\tau)$ is uniformly bounded on $[s, t]$, so the nth term on the right is bounded by

$$\frac{|t - s|^n}{n!} \left(\sup_{\tau \in [s, t]} \|H(\tau)\| \right)^n \|\varphi\|$$

so the series on the right converges in the uniform operator topology to $U(t, s)$. Thus $U(t, s)$ is jointly strongly continuous in s and t since this is true of each term on the right. It is trivial to check that $U(t, t) = I$ and that $U(t, s)^* = U(s, t)$; the formula $U(r, s)U(s, t) = U(r, t)$ is proven by multiplying out the series as in the case of unitary groups generated by bounded operators. Thus,

$$U(s, t)U(s, t)^* = I = U(s, t)^*U(s, t)$$

so $U(t, s)$ is unitary. The first statement in (X.128) follows by differentiating the series for $U(t, s)$ term by term and noting that the resulting series converges uniformly. ▮

We remark that the self-adjointness of the $H(t)$ was used only in proving that $U(t, s)$ is unitary; without self-adjointness we can still define $U(t, s)$ as before and use it to construct strong solutions $\varphi_s(t)$.

Although the Dyson expansion requires that $H(t)$ be bounded, by passing to the "interaction representation" we can use it to handle certain cases of the form

$$H(t) = H_0 + V(t)$$

where H_0 is a (possibly unbounded) self-adjoint operator and $t \to V(t)$ satisfies the hypotheses of Theorem X.69. Define

$$\tilde{V}(t) = e^{iH_0 t} V(t) e^{-iH_0 t}$$

Then $t \to \tilde{V}(t)$ also satisfies the hypotheses of Theorem X.69; we denote the corresponding propagator by $\tilde{U}(t, s)$. If we now set

$$U(t, s) = e^{-itH_0}\tilde{U}(t, s)e^{isH_0}$$

then, at least *formally*, $U(t, s)$ satisfies

$$\begin{aligned} \frac{d}{dt} U(t, s) &= -iH_0 e^{-itH_0}\tilde{U}(t, s)e^{isH_0} + e^{-itH_0}(-i\tilde{V}(t))\tilde{U}(t, s)e^{isH_0} \\ &= (-iH_0 - iV(t))U(t, s) \end{aligned}$$

so $\varphi_s(t) = U(t, s)\psi$ should be a strong solution of

$$\frac{d}{dt}\varphi_s(t) = -i(H_0 + V(t))\varphi_s(t), \qquad \varphi_s(s) = \psi$$

The difficulty is that $H_0 U(t, s)\psi = H_0 e^{-itH_0}\tilde{U}(t, s)e^{isH_0}\psi$ may not make sense since $\tilde{U}(t, s)\psi$ may not be in the domain of H_0 even if ψ is. It can be shown (Problem 66) that if $t \to [H_0, V(t)]$ is strongly continuous, then

$\varphi_s(t)$ is in fact a strong solution. This hypothesis is a special case of the more general hypotheses in Theorem X.70 (below); these give rise to strong solutions, so we will not pursue this problem further here. However, we note that for any $\psi \in \mathscr{H}$, $\psi_s(t) = e^{-iH_0 t}\tilde{U}(t, s)e^{isH_0}\psi$ is always a "weak" solution in the sense that for any $\eta \in D(H_0)$, $(\eta, \psi_s(t))$ is differentiable and

$$\frac{d}{dt}(\eta, \psi_s(t)) = -i(H_0\eta, \psi_s(t)) - i(V(t)\eta, \psi_s(t))$$

Example 1 The Dyson expansion is important for practical calculations also. Suppose that H_0 is the Hamiltonian of a quantum system and that ψ_k and ψ_ℓ are eigenfunctions of H_0 with corresponding eigenvalues λ_k and λ_ℓ. If the system starts out in state ψ_k, it will stay in ψ_k in the absence of any external potential since $e^{itH_0}\psi_k = e^{it\lambda_k}\psi_k$. However, if an external potential $V(t)$ is turned on for a while the dynamics is given by $e^{-itH_0}\tilde{U}(t, 0)\psi_k$, and if we look at the system at time t the probability that the system will be observed in state ψ_ℓ is $|(\psi_\ell, e^{-itH_0}\tilde{U}(t, 0)\psi_k)|^2$, the transition probability from ψ_k to ψ_ℓ. Using the Dyson expansion we have

$$(\psi_\ell, e^{-itH_0}\tilde{U}(t, 0)\psi_k) = (\psi_\ell, e^{-itH_0}\psi_k) - i\int_0^t (\psi_\ell, e^{-iH_0 t}\tilde{V}(t_1)\psi_k)\, dt_1 + \cdots$$

$$= -i\int_0^t e^{-i\lambda_\ell t}e^{-i(\lambda_k - \lambda_\ell)t_1}(\psi_\ell, V(t_1)\psi_k)\, dt_1 + O(t^2)$$

The constant in the term of order t^2 can be easily bounded by estimating the tail of the Dyson expansion, so for small t the above expression allows one to compute upper and lower bounds on the transition probabilities. The reader is asked to compute a specific example in Problem 67.

We come now to the main theorem in this section. Since the proof is the same in the case where $A(t)$ generates a contraction semigroup on a Banach space X, we give the proof in this more general setting. The idea of the proof is very simple and direct. For each positive integer k, we define an approximate propagator $U_k(s, t)$ on $0 \le s \le t \le 1$ by

$$U_k(t, s) = \exp\left(-(t - s)A\left(\frac{i-1}{k}\right)\right) \quad \text{if} \quad \frac{i-1}{k} \le s \le t \le \frac{i}{k} \quad (\text{where } 1 \le i \le k) \qquad (X.130a)$$

and

$$U_k(t, r) = U_k(t, s)U_k(s, r) \qquad \text{if} \quad 0 \le r \le s \le t \le 1 \qquad (X.130b)$$

That is, $U_k(t, s)$ is defined by the constant generator $A((i-1)/k)$ for s and t in the small intervals $[(i-1)/k, i/k]$ and by the product formula when s and t are not both in the same small interval. We will show that under suitable hypotheses, $U_k(t, s)$ converges to a propagator $U(t, s)$ so that $\varphi_s(t) = U(t, s)\psi$ solves $d\varphi_s(t)/dt = -A(t)\varphi_s(t)$. To see what these hypotheses should be we compute formally

$$\begin{aligned}(U_k(t, 0) - U_n(t, 0))A(0)^{-1}\varphi &= [U_n(t, s)U_k(s, 0)A(0)^{-1}\varphi]_{s=0}^{s=t} \\ &= \int_0^t \frac{d}{ds}(U_n(t, s)U_k(s, 0)A(0)^{-1}\varphi)\, ds \\ &= \int_0^t U_n(t, s)\left\{A\left(\frac{[ns]}{n}\right) - A\left(\frac{[ks]}{k}\right)\right\} \\ &\quad \times A\left(\frac{[ks]}{k}\right)^{-1} A\left(\frac{[ks]}{k}\right) U_k(s, 0)A(0)^{-1}\varphi\, ds\end{aligned} \tag{X.131}$$

where $[r]$ always denotes the largest integer less than or equal to r. The fact that $A([ns]/n)$ can be written to the right of $U_n(t, s)$ follows by writing $U_n(t, s)$ as a product if t and s are not in the same small interval. Thus to show that the left-hand side of (X.131) is small, it suffices that $A(t)A(s)^{-1} - I$ be small when $|t - s|$ is small and that $A(t)U_k(t, 0)A(s)^{-1}$ be bounded. We thus define

$$C(t, s) = A(t)A(s)^{-1} - I$$

and state:

Theorem X.70 Let X be a Banach space and let I be an open interval in $\mathbb{R}$. For each $t \in I$, let $A(t)$ be the generator of a contraction semigroup on X so that $0 \in \rho(A(t))$ and

(a) The $A(t)$ have a common domain D (from which it follows by the closed graph theorem that $A(t)A(s)^{-1}$ is bounded).

(b) For each $\varphi \in X$, $(t-s)^{-1}C(t, s)\varphi$ is uniformly strongly continuous and uniformly bounded in s and t for $t \neq s$ lying in any fixed compact subinterval of I.

(c) For each $\varphi \in X$, $C(t)\varphi \equiv \lim_{s \uparrow t} (t-s)^{-1}C(t, s)\varphi$ exists uniformly for t in each compact subinterval and $C(t)$ is bounded and strongly continuous in t.

Then for all $s \leq t$ in any compact subinterval of I and any $\varphi \in X$,

$$U(t, s)\varphi = \lim_{k\to\infty} U_k(t, s)\varphi$$

exists uniformly in s and t. Further, if $\psi \in D$, then $\varphi_s(t) \equiv U(t, s)\psi$ is in D for all t and satisfies

$$\frac{d}{dt}\varphi_s(t) = -A(t)\varphi_s(t), \qquad \varphi_s(s) = \psi$$

and $\|\varphi_s(t)\| \le \|\psi\|$ for all $t \ge s$.

We make two remarks. First, the hypothesis that $0 \in \rho(A(t))$ is usually not a strong restriction. If we can find a $z_0 \in \rho(A(t))$ for all t and if the operators $B(t) = A(t) - z_0$ satisfy the hypothesis, then $\tilde{U}(t, s) = U(t, s)e^{(s-t)z_0}$ is a propagator for $A(t)$ if $U(t, s)$ is the propagator for $B(t)$. In particular, when $A(t)$ is i times a self-adjoint operator, we can use this trick. Secondly, it is sufficient to prove the existence of the propagator for $s, t \in [0, 1]$ since we can then use the same procedure to extend to $[1, 2]$ and so forth. We begin by showing that the hypotheses imply the boundedness of $A(t)U(t, s)A(s)^{-1}$.

Lemma For $s, t \in [0, 1]$ define $W_k(t, s) = A(t)U_k(t, s)A(s)^{-1}$. Then $\|W_k(t, s)\| \le M_1$ independent of s, t, and k.

Proof Fix s, t, and k. Since $U_k(t, s)\colon D \to D$, $W_k(t, s)$ is well defined on X. Letting $\psi \in X$, we write $W_k(t, s)$ as

$$\begin{aligned}
W_k(t, s)\psi &= A(t)U_k\left(t, \frac{[kt]}{k}\right)U_k\left(\frac{[kt]}{k}, \frac{[kt]-1}{k}\right)\cdots U_k\left(\frac{[ks]+1}{k}, s\right)A(s)^{-1}\psi \\
&= A(t)A\left(\frac{[kt]}{k}\right)^{-1}U_k\left(t, \frac{[kt]}{k}\right)A\left(\frac{[kt]}{k}\right)A\left(\frac{[kt]-1}{k}\right)^{-1}\cdots \\
&\quad \times A\left(\frac{[ks]}{k}\right)^{-1}U_k\left(\frac{[ks]+1}{k}, s\right)A\left(\frac{[ks]}{k}\right)A(s)^{-1}\psi \\
&= \left(I + C\left(t, \frac{[kt]}{k}\right)\right)\left\{U_k(t, s) + \sum_{ku=[ks]+1}^{[kt]} U_k(t, u)C\left(u, u - \frac{1}{k}\right)U_k(u, s)\right. \\
&\quad + \sum_{kv=[ks]+1}^{[kt]} U_k(t, v)C\left(v, v - \frac{1}{k}\right)\sum_{ku=[ks]+1}^{[kt]} U_k(v, u) \\
&\quad \left.\times C\left(u, u - \frac{1}{k}\right)U_k(u, s) + \cdots\right\}\left(I + C\left(\frac{[ks]}{k}, s\right)\right)\psi \\
&= \left(I + C\left(t, \frac{[tk]}{k}\right)\right)\{U_k(t, s) + W_k^1(t, s) + W_k^2(t, s) + \cdots\} \\
&\quad \times \left(I + C\left(\frac{[ks]}{k}, s\right)\right)\psi
\end{aligned}$$

where

$$W_k^1(t, s) = \sum_{ku=[ks]+1}^{[kt]} U_k(t, s)C\left(u, u - \frac{1}{k}\right)U_k(u, s)$$

and

$$W_k^{m+1}(t, s) = \sum_{ku=[ks]+1}^{[kt]} U_k(t, s)C\left(u, u - \frac{1}{k}\right)W_k^m(u, s) \qquad \text{(X.132)}$$

Let

$$M_2 = \sup_{t \neq s} \|(t - s)^{-1}C(t, s)\|$$

Then

$$\left\|C\left(u, u - \frac{1}{k}\right)\psi\right\| \leq \frac{M_2}{k} \|\psi\|$$

so from (X.132) we have

$$\|W_k^1(t, s)\psi\| \leq (t - s)M_2\|\psi\| \qquad \text{and} \qquad \|W_k^m(t, s)\psi\| \leq \frac{(t - s)^m}{m!} M_2^m\|\psi\|$$

Therefore

$$\|W_k(t, s)\| \leq \left(1 + \frac{M_2}{k}\right)^2\left(1 + \sum_{m=1}^{\infty} \frac{(t - s)^m}{m!} M_2^m\right)\|\psi\|$$

We have repeatedly used the fact that $\|U_k(r_1, r_2)\psi\| \leq \|\psi\|$ since each $A(t)$ generates a contraction semigroup. ∎

Proof of Theorem X.70 Let $\varphi \in D$. Since $U_k(r, s)\varphi \in D$ for $r \geq s$ and

$$U_k(t, s)\varphi = e^{-(t-[kt]/k)A([kt]/k)}U_k\left(\frac{[kt]}{k}, s\right)\varphi$$

we see that $U_k(t, s)$ is strongly differentiable in t except when $t = j/k$, and letting $A(0)\varphi = \psi$,

$$\begin{aligned}\frac{d}{dt} U_k(t, s)\varphi &= -A\left(\frac{[kt]}{k}\right)U_k(t, s)\varphi \\ &= -A\left(\frac{[kt]}{k}\right)A(t)^{-1}A(t)U_k(t, s)A(s)^{-1}A(s)A(0)^{-1}\psi \\ &= -A\left(\frac{[kt]}{k}\right)A(t)^{-1}W_k(t, s)A(s)A(0)^{-1}\psi\end{aligned}$$

Thus, since $\|W_k(t, s)\|$ is uniformly bounded and $C(t, s)$ is strongly continuous, we see that $dU_k(t, s)\varphi/dt$ is bounded and strongly continuous except at $t = j/k$. A similar proof shows that the same conclusion holds for

$$\frac{d}{ds} U_k(t, s)\varphi = -U_k(t, s)A\left(\frac{[ks]}{k}\right)\varphi$$

when $s \neq j/k$. Thus if $k > n$,

$$\begin{aligned}
(U_k(t, s) - U_n(t, s))A(0)^{-1}\psi \\
&= [U_n(t, r)U_k(r, s)]_{r=s}^{r=t} A(0)^{-1}\psi \\
&= \int_s^t \frac{d}{dr}\{U_n(t, r)U_k(r, s)A(0)^{-1}\psi\}\, dr \qquad\qquad \text{(X.133)} \\
&= \int_s^t U_n(t, r)\left\{A\left(\frac{[rn]}{n}\right) - A\left(\frac{[rk]}{k}\right)\right\}A\left(\frac{[rn]}{n}\right)^{-1} A\left(\frac{[rn]}{n}\right) U_k(r, s)A(0)^{-1}\psi\, dr \\
&= \int_s^t U_n(t, r)C\left(\frac{[rn]}{n}, \frac{[rk]}{k}\right)\left\{1 + C\left(\frac{[rn]}{n}, r\right)\right\}W_k(r, s)\{1 + C(s, 0)\}\psi\, dr
\end{aligned}$$

Since

$$\left\|C\left(\frac{[rk]}{k}, \frac{[rn]}{n}\right)\right\| \leq 2\left|\frac{[rk]}{k} - \frac{[rn]}{n}\right| \sup_{s \neq t}|t - s|^{-1}\|C(t, s)\|$$

and $U_n(t, r)$, $C([rn]/n, r)$, $C(s, 0)$, and $W_k(r, s)$ (by the lemma) are all uniformly bounded independent of r, s, t, n, and k, we see that the strong limit of $U_k(t, s)$ exists uniformly in t and s. Since $U_k(t, s)$ is uniformly bounded

$$U(t, s)\varphi \equiv \lim_{k \to \infty} U_k(t, s)\varphi$$

exists for all $\varphi \in X$ and $U(t, s)$ is a bounded-operator-valued function and is uniformly strongly jointly continuous. We remark that the integral (X.133) is really a sum of integrals over the intervals where the derivative exists.

A similar proof shows that

$$W(t, s)\varphi \equiv \lim_{k \to \infty} W_k(t, s)\varphi$$

exists boundedly and uniformly in t and s and that $W(t, s)$ is a bounded-operator-valued function which is jointly strongly continuous. Thus, if $\varphi \in D$, $U_k(t, s)\varphi \to U(t, s)\varphi$ and

$$\begin{aligned}
A(t)U_k(t, s)\varphi &= W_k(t, s)A(s)\varphi \\
&\xrightarrow[k \to \infty]{} W(t, s)A(s)\varphi
\end{aligned}$$

Since $A(t)$ is closed, this implies that $U(t, s)\varphi \in D$ and $A(t)U(t, s)\varphi = W(t, s)A(s)\varphi$. Furthermore

$$\begin{aligned} U(t, s)\varphi - \varphi &= \lim_{k\to\infty} (U_k(t, s)\varphi - \varphi) \\ &= \lim_{k\to\infty} \int_s^t \frac{d}{dr} U_k(r, s)\varphi \, dr \\ &= \lim_{k\to\infty} -\int_s^t A\left(\frac{[rk]}{k}\right) U_k(r, s)\varphi \, dr \\ &= -\lim_{k\to\infty} \int_s^t A\left(\frac{[rk]}{k}\right) A(r)^{-1} A(r) U_k(r, s) A(s)^{-1} A(s)\varphi \, dr \\ &= -\int_s^t W(r, s)A(s)\varphi \, dr \end{aligned}$$

Since $W(r, s)$ is strongly continuous,

$$\frac{d}{dt} U(t, s)\varphi = -W(t, s)A(s)\varphi = -A(t)U(t, s)\varphi$$

which concludes the proof of Theorem X.70. ∎

Example 2 We can easily apply this result to the heat equation with time-dependent sources and sinks proportional to the temperature. Let $q(x, t)$ be a bounded real-valued continuously differentiable function on $\mathbb{R}^{n+1}$ so that $\partial q(x, t)/\partial t$ is bounded. Let M be the bound of q and set

$$A(t) = -\Delta + q(x, t) + (M + 1)$$

on $C_\infty(\mathbb{R}^n)$. From Examples 3 and 4 in Section X.8 we know that $A(t)$ is the generator of a contraction semigroup on $C_\infty(\mathbb{R}^n)$ and that $D(A(t)) = D(-\Delta)$ for all t. The reader can easily check (Problem 68) that the hypotheses on $q + M + 1$ imply that the conditions of Theorem X.70 are satisfied. Thus for each $\psi \in D(-\Delta)$ there is a function $\tilde{\varphi}(x, t)$ so that for each t, $\tilde{\varphi}(x, t) \in D(-\Delta)$ and

$$\frac{d}{dt} \tilde{\varphi}(x, t) = \Delta\tilde{\varphi}(x, t) - q(x, t)\tilde{\varphi}(x, t) - (M + 1)\tilde{\varphi}(x, t)$$

$$\tilde{\varphi}(x, 0) = \psi(x)$$

If we now define $\varphi(x, t) = e^{(M+1)t}\tilde{\varphi}(x, t)$, then $\varphi(x, t)$ satisfies

$$\frac{d}{dt} \varphi(x, t) = \Delta\varphi(x, t) - q(x, t)\varphi(x, t)$$

$$\varphi(x, 0) = \psi(x)$$

Notice that $U_k(t, s)$ is positivity preserving for each k since it is the product of positivity-preserving transformations (see Example 4 in Section X.8). Thus $U(t, s)$ is positivity preserving since it is the strong limit of the $U_k(t, s)$. Therefore, given any nonnegative initial data $\psi \in C_\infty(\mathbb{R})$, the solution $\varphi(x, t) = e^{(M+1)t}U(t, s)\psi$ will remain nonnegative corresponding to our intuition about heat flow.

Finally, we apply Theorem X.70 to the quantum mechanical case.

Theorem X.71 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and suppose that $t \to V_1(t)$ and $t \to V_2(t)$ are continuously differentiable $L^2(\mathbb{R}^3)$-valued and $L^\infty(\mathbb{R}^3)$-valued functions respectively. Let $V(t) = V_1(t) + V_2(t)$ and set $H(t) = H_0 + V(t)$. Then there is a unitary propagator $U(t, s)$ on $L^2(\mathbb{R}^3)$ so that for each $\psi \in D(H_0)$, $\varphi_s(t) = U(t, s)\psi$ is strongly differentiable and satisfies

$$\frac{d}{dt}\varphi_s(t) = -iH(t)\varphi_s(t), \qquad \varphi_s(s) = \psi \tag{X.134}$$

Proof We will construct a unitary propagator for each finite interval $[-T, T]$. By Theorem X.15, $H_0 + V(t)$ is self-adjoint on $D(-\Delta)$ for each t. Further, since $V_1(t)$ and $V_2(t)$ are uniformly bounded in L^2 and L^∞ norm respectively, we can find a constant $D \geq 0$ so that $H_0 + V(t) + D \geq \frac{1}{2}$ for all $t \in [-T, T]$. Thus $i(H_0 + V(t) + D)$ and $-i(H_0 + V(t) + D)$ generate contraction semigroups for each t and $(\pm i(H_0 + V(t) + D))^{-1}$ exists for $t \in [-T, T]$. Further, the hypotheses on $t \to V_1(t)$ and $t \to V_2(t)$ imply that $i(H_0 + V(t) + D)$ and $-i(H_0 + V(t) + D)$ satisfy the hypotheses (b) and (c) of Theorem X.70. Let $U^+(t, s)$ and $U^-(t, s)$ be the corresponding propagators. Since U_k^+ and U_k^- are unitary for each k, U^+ and U^- are unitary. Now define

$$\tilde{U}(t, s) = \begin{cases} U^+(t, s), & s \leq t \\ U^-(s, t), & t \leq s \end{cases}$$

and

$$U(t, s) = e^{iD(t-s)}\tilde{U}(t, s) \ \blacksquare$$

We conclude this section with a brief outline of a method due to J. Howland for turning time-dependent problems into time-independent problems. In classical mechanics, Hamilton's equations for a system with Hamiltonian function $H(p_1, \ldots, p_n, q_1, \ldots, q_n, t)$ are

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad -\frac{dp_i}{dt} = \frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n \tag{X.135}$$

If H depends on t, energy is not conserved by such a system, but we can set up a corresponding energy conserving system by introducing t as a coordinate and the energy E of the external source as its conjugate momentum. The new Hamiltonian is

$$h(\mathbf{p}, \mathbf{q}, t, E) = E + H(\mathbf{p}, \mathbf{q}, t)$$

so if we denote by σ the new time variable, Hamilton's equations read

$$\begin{aligned} \frac{dq_i}{d\sigma} &= \frac{\partial H}{\partial p_i}, \qquad -\frac{dp_i}{d\sigma} = \frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n \\ \frac{dt}{d\sigma} &= \frac{\partial h}{\partial E} = 1, \qquad -\frac{dE}{d\sigma} = \frac{\partial H}{\partial t} \end{aligned} \tag{X.136}$$

This set of equations is equivalent to (X.135).

We can reformulate the quantum-mechanical problem similarly. Let $H(t)$ be a family of self-adjoint operators on a Hilbert space $\mathscr{H}$ and set $\mathscr{H}_1 = L^2(\mathbb{R}; \mathscr{H})$, the Hilbert space of strongly measurable $\mathscr{H}$-valued functions $f(\cdot)$ on $\mathbb{R}$ such that $\int_{-\infty}^{\infty} \|f(t)\|_{\mathscr{H}}^2 \, dt < \infty$. If we now define h on $\mathscr{H}_1$ by

$$(hf)(t) = -i\frac{d}{dt}f(t) + H(t)f(t)$$

there should be (according to the classical analogy) a correspondence between the solutions of

$$\frac{d}{d\sigma}\varphi(\sigma) = -ih\varphi(\sigma)$$

on $\mathscr{H}_1$ and the solutions of the time-dependent problem (X.134) on $\mathscr{H}$. Suppose that $U(t, s)$ is a unitary propagator on $\mathscr{H}$. Then

$$(\hat{U}(\sigma)f)(t) \equiv U(t, t-\sigma)f(t-\sigma) \tag{X.137}$$

is a strongly continuous unitary group on $\mathscr{H}_1$ (Problem 69). Notice that this means that if T_σ is the group on $\mathscr{H}_1$ which acts by $(T_\sigma f)(t) = f(t+\sigma)$, then $\hat{U}(\sigma)T_\sigma$ acts on $\mathscr{H}_1$ by multiplication by an operator-valued function. Conversely, one can prove that to each strongly continuous unitary group $\hat{U}(\sigma)$ on $\mathscr{H}$, so that $\hat{U}(\sigma)T_\sigma$ is multiplication by an operator-valued function, there corresponds a unique unitary propagator $U(t, s)$ on $\mathscr{H}$ so that (X.137) holds. Thus, we have a correspondence between unitary propagators on $\mathscr{H}$ and certain strongly continuous one-parameter unitary groups on $\mathscr{H}_1$. Notice that $\hat{U}(\sigma)$ will always be strongly differentiable on a dense set in $\mathscr{H}_1$ by Stone's theorem, but that $U(t, s)$ need not be strongly differentiable on $\mathscr{H}$. Thus, we have a method of proving the existence of propagators in situations where we might not expect strong differentiability, i.e., situations where we cannot use Theorem X.70. This propagator formally solves

$$\frac{d}{dt} U(t, s)\psi = -iH(t)U(t, s)\psi$$

Example 3 We will consider again the case $H(t) = H_0 + V(t)$ where H_0 is a self-adjoint operator on $\mathscr{H}$ and $t \to V(t)$ is a strongly continuous map from $\mathbb{R}$ to the bounded operators on $\mathscr{H}$. To make things easier, we will assume that $\|V(t)\|$ is uniformly bounded on all of $\mathbb{R}$. As before we let $\tilde{V}(t) = e^{iH_0t}V(t)e^{-iH_0t}$. Let $\hat{\tilde{V}}$ be the operator on $L^2(\mathbb{R}; \mathscr{H})$ which acts by $(\hat{\tilde{V}}f)(t) = \tilde{V}(t)f(t)$ and let $C_0^1(\mathbb{R}; \mathscr{H})$ denote the continuously differentiable $\mathscr{H}$-valued functions on $\mathbb{R}$ with compact support. Then it is not hard to check that $i^{-1}\, d/dt$ is essentially self-adjoint on $C_0^1(\mathbb{R}; \mathscr{H})$. Since $\hat{\tilde{V}}$ is a bounded operator, $i^{-1}\, d/dt + \hat{\tilde{V}}$ is also essentially self-adjoint on $C_0^1(\mathbb{R}; \mathscr{H})$ and it is possible to show that $\exp(-i\sigma(i^{-1}\, d/dt + \hat{\tilde{V}}))T_\sigma$ operates by multiplication by an operator-valued function. Thus by the correspondence theorem mentioned above, there is a strongly continuous propagator $\tilde{U}(t, s)$ on $\mathscr{H}$ so that

$$\left(\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)f\right)(t) = \tilde{U}(t, t-\sigma)f(t-\sigma)$$

One can easily check that this $\tilde{U}$ is just the propagator arising from applying the Dyson expansion to $t \to \tilde{V}(t)$. Now, let $\hat{W}$ act on $L^2(\mathbb{R}; \mathscr{H})$ by $(\hat{W}f)(t) = e^{-iH_0t}f(t)$. Then $\hat{W}$ is unitary so

$$\hat{W}\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)\hat{W}^{-1}$$

is again a strongly continuous unitary group on $L^2(\mathbb{R}; \mathscr{H})$ and clearly

$$\left(\hat{W}\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)\hat{W}^{-1}f\right)(t) = e^{-itH_0}\tilde{U}(t, t-\sigma)e^{i(t-\sigma)H_0}f(t-\sigma)$$

So $U(t, s) = e^{-itH_0}\tilde{U}(t, s)e^{isH_0}$ is the propagator on $\mathscr{H}$ which formally solves

$$\frac{d}{dt} U(t, s) = -i(H_0 + V(t))U(t, s)$$

since the generator of $\hat{W}\exp(-i\sigma(i^{-1}\, d/dt + \hat{\tilde{V}}))\hat{W}^{-1}$ is $i^{-1}d/dt + H_0 + \hat{V}$.