APPPHYS383 Tuesday 12 January 2010

Background material: Picard's method of successive approximations

[L. Perko, *Differential Equations and Dynamical Systems* (Springer-Verlag, New York, 2001)]
Consider an ordinary differential equation,

$$\dot{x} = f(x), \quad x(0) = x_0,$$

where x and f may here be scalar or vector-valued. If we formally integrate both sides we obtain

$$\int_0^t dx = \int_0^t f(x(s))ds,$$

$$x(t) - x_0 = \int_0^t f(x(s))ds,$$

$$x(t) = x_0 + \int_0^t f(x(s))ds,$$

which simply converts our original differential equation into an integral one. The integral version can be tackled using the method of successive approximations,

$$u_0(t) = x_0,$$

$$u_{k+1}(t) = x_0 + \int_0^t f(u_k(s))ds.$$

It can be shown rigorously that for reasonable functions $f(\cdot)$ (f and its first derivative must be continuous on an open interval containing x_0), the sequence limit function

$$u(t) = \lim_{k\to\infty} u_k(t),$$

exists and satisfies the integral equation

$$u(t) = x_0 + \int_0^t f(u(s))ds.$$

We can thus expect that $u_k(t)$ for sufficiently large k provides a good approximation to the solution of $\dot{x} = f(x)$.

As an illustrative example we can consider

$$\dot{x} = x^2, \quad x(0) = 1,$$

(although we should be careful about interval of existence). The first few successive approximations are:

$$u_0(t) = 1,$$

$$u_1(t) = 1 + \int_0^t f(1)ds = 1 + t,$$

$$u_2(t) = 1 + \int_0^t f(1+s)ds = 1 + \int_0^t (1 + 2s + s^2)ds = 1 + t + t^2 + \frac{1}{3}t^3,$$

$$u_3(t) = 1 + \int_0^t \left(1 + s + s^2 + \frac{1}{3}s^3\right)^2 ds$$

$$= 1 + t + t^2 + t^3 + \frac{2}{3}t^4 + \frac{1}{3}t^5 + \frac{1}{9}t^6 + \frac{1}{63}t^7.$$

On the time interval $t \in (-\infty, 1)$ we can actually identify an exact solution to the ODE,

$$x(t) = \frac{1}{1-t},$$

since

$$\frac{d}{dt}\left(\frac{1}{1-t}\right) = (1-t)^{-2} = x^2(t),$$

and $x(0) \to 1$. If we examine the Taylor expansion of this solution about $t = 0$,

$$x(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} f^{(n)}(0),$$

we have

$$f^{(n)}(t) = n!(1-t)^n,$$

and hence

$$x(t) = 1 + t + t^2 + t^3 + \cdots,$$

and we can directly see the correspondence with the successive approximations ($u_k(t)$ appears good to order k in t).

Successive approximations for the Schrödinger evolution operator

If we consider the definition of the evolution operator $U(t_f, t_i)$,

$$|\psi(t_f)\rangle = U(t_f, t_i)|\psi(t_i)\rangle,$$

where the state must satisfy the Schrödinger Equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle,$$

we find the evolution equation

$$\begin{aligned}
i\hbar \frac{d}{dt}(U(t,t_i)|\psi(t_i)\rangle) &= HU(t,t_i)|\psi(t_i)\rangle, \\
i\hbar \left(\frac{d}{dt}U(t,t_i)\right)|\psi(t_i)\rangle &= HU(t,t_i)|\psi(t_i)\rangle, \\
\frac{d}{dt}U(t,t_i) &= \frac{1}{i\hbar}HU(t,t_i), \quad U(t_i,t_i) = 1.
\end{aligned}$$

By similar reasoning as was applied above, this can be transformed into an integral equation,

$$U(t_f, t_i) = 1 + \frac{1}{i\hbar}\int_{t_i}^{t_f} HU(s,t_i)ds.$$

Of course, if the eigenstates of the total Hamiltonian are known, it is presumably possible to compute the evolution operator explicitly by exponentiation.

If on the other hand our total Hamiltonian splits into a part with known eigenstates, plus a perturbation,

$$H = H_0 + V,$$

we can choose to work in the interaction picture. The states and operators are transformed by a unitary operator

$$T(t) = \exp(iH_0(t - t_0)/\hbar),$$

according to

$$\begin{aligned}
|\psi(t)\rangle &\mapsto |\tilde{\psi}(t)\rangle = T(t)|\psi(t)\rangle, \\
A(t) &\mapsto \tilde{A}(t) = T(t)A(t)T^\dagger(t).
\end{aligned}$$

In the interaction picture we have the Schrödinger Equation

$$\begin{aligned}
i\hbar \frac{d}{dt}|\psi(t)\rangle &= H|\psi(t)\rangle, \\
i\hbar \frac{d}{dt}(T^\dagger(t)|\tilde{\psi}(t)\rangle) &= H(T^\dagger(t)|\tilde{\psi}(t)\rangle), \\
i\hbar \left(\frac{d}{dt}T^\dagger(t)\right)|\tilde{\psi}(t)\rangle + i\hbar T^\dagger(t)\frac{d}{dt}|\tilde{\psi}(t)\rangle &= H(T^\dagger(t)|\tilde{\psi}(t)\rangle), \\
i\hbar T^\dagger(t)\frac{d}{dt}|\tilde{\psi}(t)\rangle &= -i\hbar\left(-\frac{i}{\hbar}H_0T^\dagger(t)\right)|\tilde{\psi}(t)\rangle + H(T^\dagger(t)|\tilde{\psi}(t)\rangle), \\
i\hbar \frac{d}{dt}|\tilde{\psi}(t)\rangle &= T(t)(-H_0 + H)T^\dagger(t)|\tilde{\psi}(t)\rangle, \\
i\hbar \frac{d}{dt}|\tilde{\psi}(t)\rangle &= \tilde{V}(t)|\tilde{\psi}(t)\rangle,
\end{aligned}$$

with corresponding evolution equation for the interaction picture evolution operator $\tilde{U}(t, t_i)$,

$$\begin{aligned}
|\tilde{\psi}(t)\rangle &= \tilde{U}(t,t_i)|\tilde{\psi}(t_i)\rangle, \\
i\hbar \frac{d}{dt}(\tilde{U}(t,t_i)|\tilde{\psi}(t_i)\rangle) &= \tilde{V}(t)\tilde{U}(t,t_i)|\tilde{\psi}(t_i)\rangle, \\
\frac{d}{dt}\tilde{U}(t,t_i) &= \frac{1}{i\hbar}\tilde{V}(t)\tilde{U}(t,t_i),
\end{aligned}$$

and integral form

$$\tilde{U}(t_f, t_i) = 1 + \frac{1}{i\hbar}\int_{t_i}^{t_f} \tilde{V}(s)\tilde{U}(s,t_i)ds.$$

We can now apply Picard's method of successive approximations, with

$$\begin{aligned}
\tilde{U}_0(t_f, t_i) &= 1, \\
\tilde{U}_{k+1}(t_f, t_i) &= 1 + \frac{1}{i\hbar}\int_{t_i}^{t_f} \tilde{V}(s)\tilde{U}_k(s,t_i)ds.
\end{aligned}$$

Hence

$$
\begin{aligned}
\tilde{U}_1(t_f,t_i) &= 1+\frac{1}{i\hbar}\int_{t_i}^{t_f}\tilde{V}(s_1)ds_1,\\
\tilde{U}_2(t_f,t_i) &= 1+\frac{1}{i\hbar}\int_{t_i}^{t_f}\tilde{V}(s_2)\left\{1+\frac{1}{i\hbar}\int_{t_i}^{s_2}\tilde{V}(s_1)ds_1\right\}ds_2\\
&= 1+\frac{1}{i\hbar}\int_{t_i}^{t_f}\tilde{V}(s_2)ds_2+\left(\frac{1}{i\hbar}\right)^2\int_{t_i}^{t_f}ds_2\int_{t_i}^{s_2}ds_1\tilde{V}(s_2)\tilde{V}(s_1),\\
&\ \ \vdots
\end{aligned}
$$

which may be directly compared with Eqs. (14.a,b) in Complement A_I. As is discussed there, such an expansion leads directly to perturbative methods for computing transition amplitudes.