Solving the Schrödinger equation

This application note describes how to solve the time independent Schrödinger equation for a nonrelativistic particle

\[
\left[-\frac{\hbar}{2m} \nabla^2 + V(x)\right] \Psi(x) = E \Psi(x) \tag{1}
\]

in one dimension on an analog computer. It is based on an article written in 1986 by my late friend Heribert Müller.\(^1\) (1) can be rearranged into

\[
-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + (V(x) - E) \Psi(x) = 0 \tag{2}
\]

with

\[
\hbar = \frac{\hbar}{2\pi}
\]

denoting the reduced Planck constant, \(m\) being the mass of the nonrelativistic particle under consideration, \(V(x)\) representing the potential energy, i.e. the depth of the potential well, \(E\) being the energy of the particle, and \(\Psi(x)\) representing the probability amplitude depending on the \(x\)-coordinate of the one-dimensional system being examined. Solving (2) for the highest derivative yields

\[
\frac{\partial^2 \Psi(x)}{\partial x^2} = \frac{2m}{\hbar} (V(x) - E) \Psi(x).
\]

To solve this problem on an analog computer, \(x\) will be represented by the integration time, basically yielding

\[
\ddot{\Psi} = \Phi \Psi \tag{3}
\]

with

\[
\Phi := \frac{2m}{\hbar} (V - E)
\]

and omitting the function arguments \((t)\) instead of \((x)\) to make the equation easier to read.

\(^1\)See [Müller 1986].
Equation (3) can be easily converted into an analog computer program as shown in figure 1. The input is the time-dependent function $\Phi$ basically describing the potential well, yielding the probability amplitude $\Psi$ as well as $\Psi^2$ as its output. The initial conditions for this function are set with the potentiometers $\dot{\Psi}_0$ and $\dot{\Psi}_0$.

The computer will be run in repetitive operation with an OP-time of 20 ms and a time scale factor of $k_0 = 10^2$ set on all integrators. The input function $\Phi$ resembles a square trough and is generated with the circuit shown in figure 2: The integrator on the left yields a linear ramp function running from $-1$ to $+1$ which is then fed to a series-connection of two comparators with electronic switches. Using the coefficient potentiometers labelled $l$ and $r$, the left and right position of the trough’s walls can be set. The height and depth of the trough are set by the coefficients $E$ and $V_0$ yielding $\Phi$.

Figure 3 shows a typical result from an unscaled simulation run.\(^2\) Here, the trough parameters $l$ and $r$ were set to yield an approximately symmetric trough which is shown in the upper trace. The two following graphs show $\Psi$ and $\Psi^2$. Here, $\dot{\Psi}_0$ was assumed to be zero while $\dot{\Psi}_0$ was set so that the two integrators in figure 1 did not go into overload.

One of the big advantages of an analog computer is the ease with which parameter

\(^2\)Scaling this problem is described in detail in [Müller 1986].
Figure 2: Generating the potential well

Figure 3: Typical solution of the Schrödinger equation
variations can be tested. Varying $E$, $V_0$, $\dot{\Psi}_0$, and $\Psi_0$ gives a good feeling of the behaviour of the one-dimensional Schrödinger equation.

References