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

$$\hbar = \frac{h}{2\pi}$$

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].

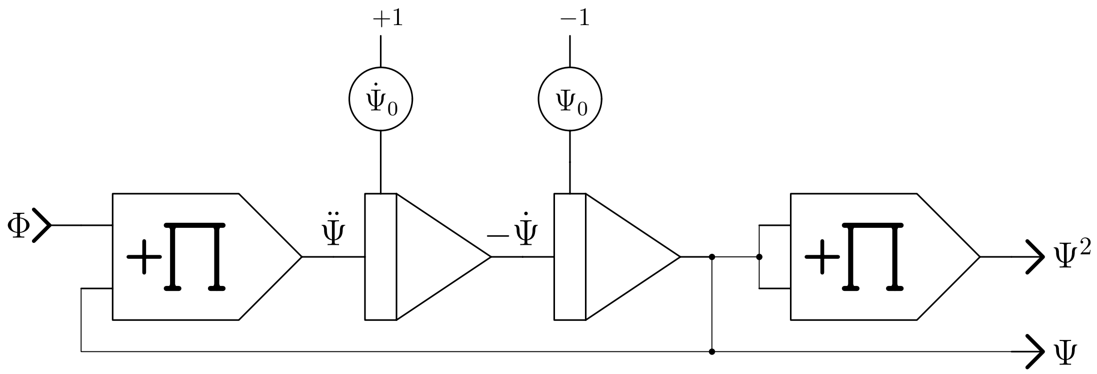

Figure 1: Setup for the one-dimensional SCHRÖDINGER equation

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

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 Ψ and Ψ^2. Here, Ψ_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].

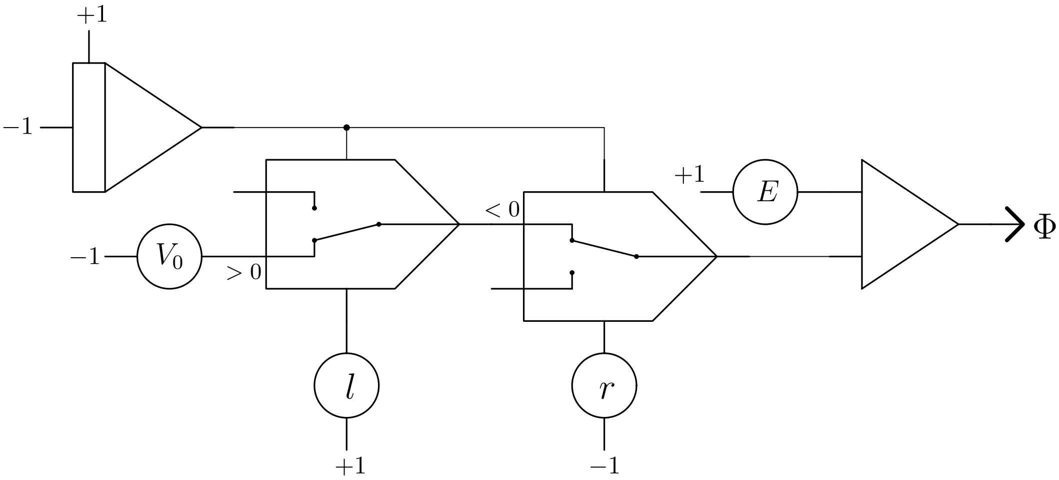

Figure 2: Generating the potential well

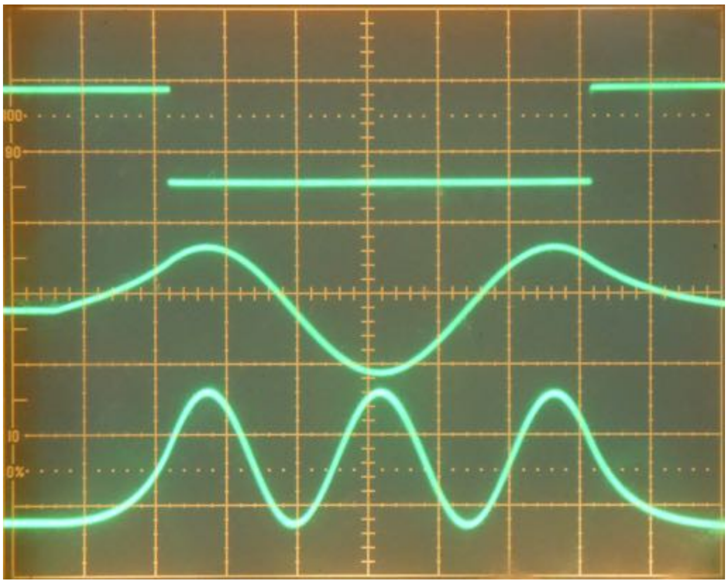

Figure 3: Typical solution of the SCHRÖDINGER equation

variations can be tested. Varying E, V_0, $\dot{\Psi}_0$, and Ψ_0 gives a good feeling of the behaviour of the one-dimensional Schrödinger equation.

References

[Müller 1986] Heribert Müller, "Simulation und Lösung physikalischer Probleme mit dem Analogrechner", in *Praxis der Naturwissenschaften, Physik*, Aulis Verlag, Heft 3/35, 15. April 1986, pp. 21–25