

Solving the SCHRÖDINGER equation

This application note describes how to solve the SCHRÖDINGER equation for a nonrelativistic particle

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

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

$$-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + (V(x) - E) \Psi(x) = 0 \quad (2)$$

with

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

denoting the reduced PLANCK constant, m being the mass of the non-relativistic 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

$$\ddot{\Psi} = \Phi \Psi \quad (3)$$

¹See [MÜLLER 1986].

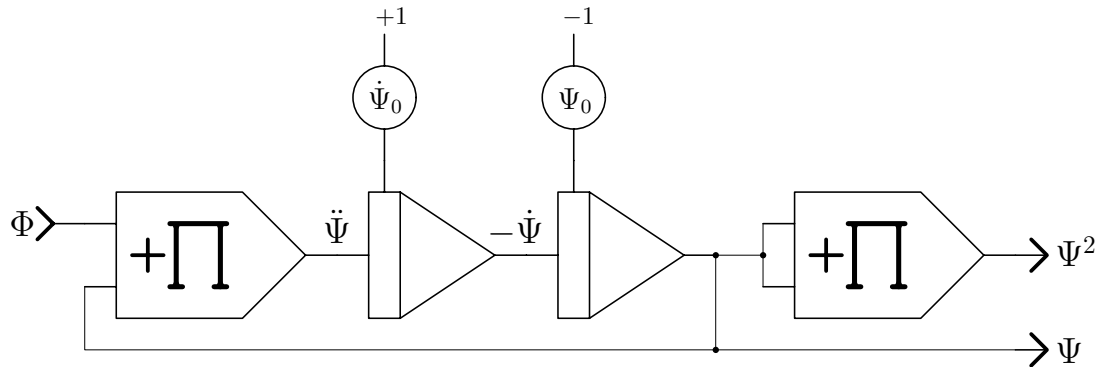


Figure 1: Setup for the one-dimensional SCHRÖDINGER equation

with

$$\Phi := \frac{2m}{\hbar}(V - E).$$

(As usual the function argument (t) is omitted for clarity.)

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 rectangular trough and is generated using 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 two comparators with electronic switches connected in series.

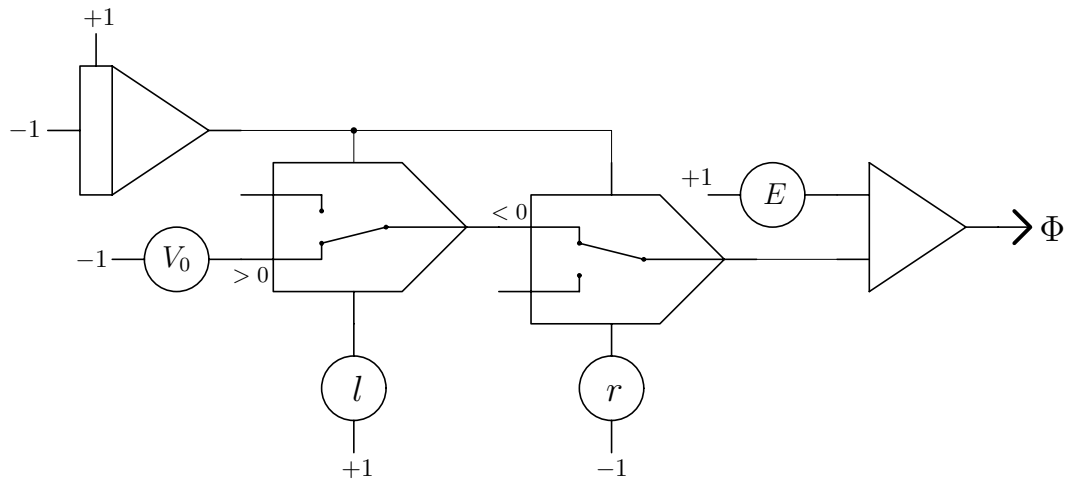


Figure 2: Generating the potential well

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 curves 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 variations can be tested. Varying E , V_0 , $\dot{\Psi}_0$, and Ψ_0 gives a good feeling of the behaviour of the system under investigation.

²Scaling this problem is described in detail in [MÜLLER 1986].

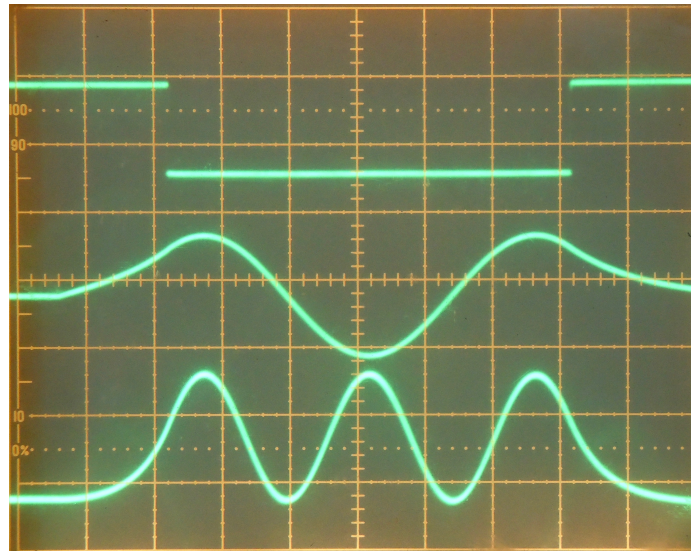


Figure 3: Typical solution of the SCHRÖDINGER equation

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