Quantum Mechanical Two-Body Problem with Gaussian potential

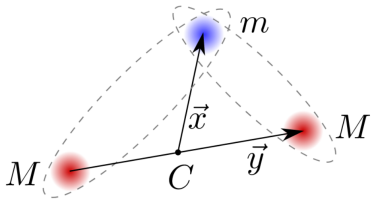

Figure 1: Two heavy (M) particles and one light (m) particle in a three-body system

This application note is inspired by the work described in [THIES et al. 2022]. In this paper the authors develop a numerical method to calculate binding energies of a quantum mechanical three-body system efficiently. This three-body system is composed of two heavy and one light particle. In figure 1 the system is displayed with its two-body (heavy/light) subsystems marked by dashed ellipses. The routine to calculate binding energies for the three-body system first solves the two-body subsystem. This application note aims to reproduce the findings in [THIES et al. 2022] for the two-body systems using an analog computer.

1 Implementation

The SCHRÖDINGER equation for the two-body system is given by ([THIES et al. 2022] eq. (1))

$$\left[-\frac{1}{2}\Delta_\xi - v_0 f(\xi)\right]\psi(\xi) = E\psi(\xi), \tag{1}$$

where ξ is the distance between the two particles, E their energy, $\psi(\xi)$ the wave function of the system, $-v_0 f(\xi)$ an attractive potential between the particles, and

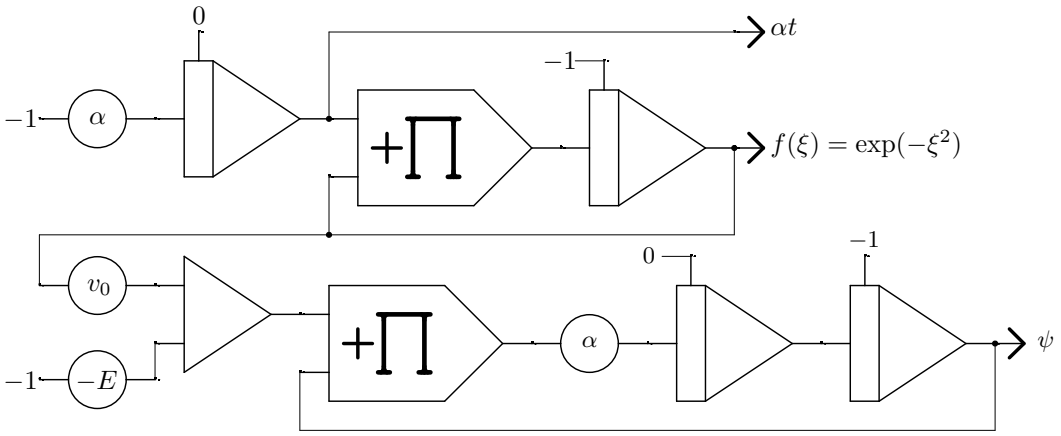

Figure 2: Analog computer program solving the SCHRÖDINGER equation with GAUSSian potential.

Δ_ξ the Laplace operator. The depth of the potential is given by v_0 and the shape is defined by a GAUSSian function

$$f(\xi) = \exp(-\xi^2). \tag{2}$$

With a GAUSSian potential eq. 1 becomes symmetric under the transformation $\xi \to -\xi$ and the solutions are either even ($\psi(\xi) = \psi(-\xi)$) or odd ($\psi(-\xi) = -\psi(\xi)$). Hence, eq. 1 can be solved for $\xi > 0$ with initial conditions of either $\psi(0) \neq 0$ and $\psi'(0) = 0$ (even) or $\psi(0) = 0$ and $\psi'(0) \neq 0$ (odd).

In figure 2 the analog program to solve eq. 1 is shown. In the upper half the GAUSSian function is generated by solving the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}\xi} f(\xi) = -2\xi f(\xi), \qquad \text{and} \qquad f(0) = 1. \tag{3}$$

One has to be careful about the variable of interest in equations such as 3 because $\frac{\mathrm{d}}{\mathrm{d}\xi} \neq \frac{\mathrm{d}}{\mathrm{d}t}$ (all integrators integrate over time).

In the following ξ is defined as $\xi = \sqrt{\frac{\alpha}{2}}t$, implying $\frac{\mathrm{d}}{\mathrm{d}\xi} = \sqrt{\frac{2}{\alpha}}\frac{\mathrm{d}}{\mathrm{d}t}$. With this eq. 3

can rewritten as

$$\sqrt{\frac{2}{\alpha}}\frac{\mathrm{d}}{\mathrm{d}t}f(\xi) = -2\sqrt{\frac{\alpha}{2}}tf(\xi)$$
$$\Leftrightarrow \frac{\mathrm{d}}{\mathrm{d}t}f(\xi) = -\alpha t f(\xi) \qquad \text{and} \qquad f(0) = 1. \tag{4}$$

The implementation of eq. 4 can directly be seen in the upper half of the analog program in figure 2. The lower half implements the two-body SCHRÖDINGER equation in eq. 1. To see this correspondence the equation can be rewritten:

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi(\xi) = -2\left[v_0 f(\xi) + E\right]\psi(\xi) \tag{5}$$
$$\Leftrightarrow \quad \left(\sqrt{\frac{2}{\alpha}}\right)^2 \frac{\mathrm{d}^2}{\mathrm{d}t^2}\psi(\xi) = -2\left[v_0 f(\xi) + E\right]\psi(\xi) \tag{6}$$
$$\Leftrightarrow \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2}\psi(\xi) = -\alpha\left[v_0 f(\xi) + E\right]\psi(\xi). \tag{7}$$

The implementation of eq. 7 in the lower half of figure 2 is straightforward. The potentiometer for E gets a negative reference input since for a positive potential depth $v_0 > 0$ the wave function ψ is only bound if the energy is negative. The initial conditions for ψ in figure 2 are set to generate even solutions.

2 Calculation

In [THIES et al. 2022] binding energies for the three-body system are calculated for values of the potential depth v_0 for which the two-body subsystem has specific energy values. So for a given energy one is interested in the value of v_0, or in other words the strength of the attractive force between the two particles, for which the two-body system is bound.

A system is in a bound state, if its wave function ψ remains localized. This implies that for large values of ξ, ψ tends to zero ($\lim_{\xi\to\pm\infty}\psi(\xi) = 0$). In the following two-

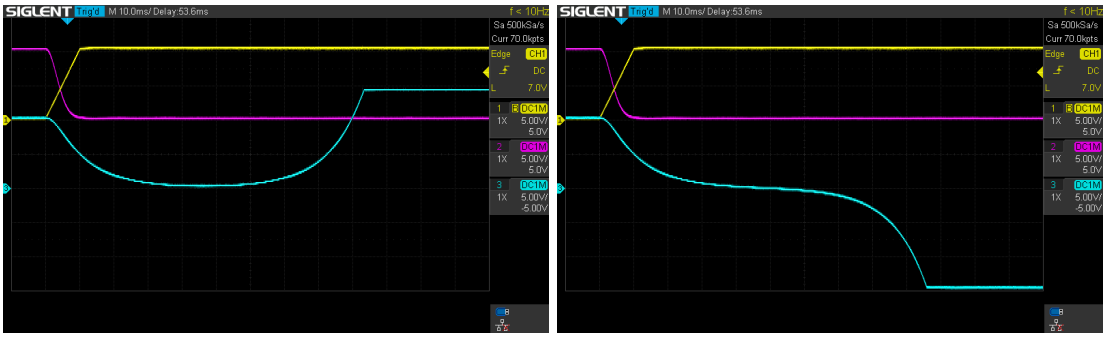

Figure 3: Two runs of the analog program for $E = -0.1$ and $\alpha = 0.1$ with αt in yellow, $f(t := \sqrt{\frac{2}{\alpha}}\xi)$ in red and $\psi(t := \sqrt{\frac{2}{\alpha}}\xi)$ in blue. The potential depth is $v_0 \approx 0.342$ for the left run and $v_0 \approx 0.343$ for the right run.

body energies of $E = -10^{-1}, -10^{-2}, -10^{-3}$ are investigated. The potential depth v_0 required for the system to be in a bound state can be derived by varying v_0 until ψ is localized.

This process in depicted in figure 3. The program is set up for $E = -0.1$ and $\alpha = 0.1$ on an Analog Paradigm Model-1. All integrators have a time scale factor of $k_0 = 10^4$ with the exception of two integrators with an $\alpha = 0.1$ scaling in front, which is absorbed into the time scale factor by setting $k_0 = 10^3$. With this setup the effect on ψ by varying v_0 can be tested and a bound state of the system can be derived.

In figure 3 it can be seen that even very slight changes of v_0 affect ψ. Both of the states are not bound states, because $\lim_{\xi \to \pm\infty} \psi(\xi) \neq 0$. However, the two states in figure 3 suggest that for some value of v_0 between 0.342 and 0.343 there is a bound state. With this process regions of v_0 for different values of E, in which the system is bound, can be derived.

E	v_0	
	Model-1	[THIES et al. 2022]
-10^{-1}	$0.343(1)$	0.34459535
-10^{-2}	$0.0886(1)$	0.08887372
-10^{-3}	$0.0250(1)$	0.02613437

Table 1: Values of v_0 at different energies E. Results from the Model-1 analog computer are compared with results from [THIES et al. 2022] table 1.

3 Results

In table 1 the results from the analog computer are compared with the results in [THIES et al. 2022]. The values of v_0 derived by the analog computer setup are all close the theoretical values. For $E = -0.1$ and $E = -0.01$ the deviations are less than 0.5% and for $E = -10^{-3}$ it is about 5%. The uncertainties given for values of v_0 from the Model-1 are derived from the variation of v_0 around the bounded state of ψ. Uncertainties of the analog program due to the limited precision of analog components are not analysed.

References

[THIES et al. 2022] JONAS THIS, MORITZ TRAVIS HOF, MATTHIAS ZIMMERMANN, MAXIM EFREMOV, "Tensor Product Scheme for Computing of Bound States of the Quantum Mechanical Three-Body Problem", `https://arxiv.org/pdf/2111.02534.pdf`, 2022