Quantum Mechanical Two-Body Problem with Gaussian potential

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))

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

where \( \xi \) 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
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Figure 2: Analog computer program solving the Schrödinger equation with Gaussian potential.

\[ \Delta \xi = \text{the Laplace operator.} \quad \text{The depth of the potential is given by } v_0 \quad \text{and the shape is defined by a Gaussian function} \]

\[ f(\xi) = \exp(-\xi^2). \] \hspace{1cm} (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

\[ \frac{d}{d\xi} f(\xi) = -2\xi f(\xi), \quad \text{and} \quad f(0) = 1. \] \hspace{1cm} (3)

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

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

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can rewritten as
\[ \sqrt{\frac{2}{\alpha}} \frac{d}{dt} f(\xi) = -2 \sqrt{\frac{\alpha}{2}} t f(\xi) \]
\[ \iff \frac{d}{dt} f(\xi) = -\alpha t f(\xi) \quad \text{and} \quad f(0) = 1. \] (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:
\[ \frac{d^2}{d\xi^2} \psi(\xi) = -2 [v_0 f(\xi) + E] \psi(\xi) \] (5)
\[ \iff \left( \frac{2}{\alpha} \right)^2 \frac{d^2}{d\xi^2} \psi(\xi) = -2 [v_0 f(\xi) + E] \psi(\xi) \] (6)
\[ \iff \frac{d^2}{dt^2} \psi(\xi) = -\alpha [v_0 f(\xi) + E] \psi(\xi). \] (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 \( \psi \) is only bound if the energy is negative. The initial conditions for \( \psi \) 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 \( \psi \) remains localized. This implies that for large values of \( \xi \), \( \psi \) tends to zero \( (\lim_{\xi \to \pm \infty} \psi(\xi) = 0) \). In the following two-
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 $\psi$ is localized.

This process is 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 $\psi$ 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 $\psi$. 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.
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.

<table>
<thead>
<tr>
<th>$E$</th>
<th>$v_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-10^{-1}$</td>
<td>0.343(1)</td>
</tr>
<tr>
<td>$-10^{-2}$</td>
<td>0.0886(1)</td>
</tr>
<tr>
<td>$-10^{-3}$</td>
<td>0.0250(1)</td>
</tr>
</tbody>
</table>

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 $\psi$. Uncertainties of the analog program due to the limited precision of analog components are not analysed.

References