1. **Delta-shell potential**
The stationary Schrödinger equation in k-space reads

$$\frac{k^2}{2\mu}\psi_n(k) + \frac{2}{\pi}\int_0^\infty {k'}^2 V(k,k')\psi_n(k')\,\mathrm{d}k' = E_n\psi_n(k), \tag{1}$$

where $V(k,k')$ is a non-local potential. Here, we want to solve this equation for the *local* delta-shell potential

$$V(r) = \frac{\lambda}{2\mu}\,\delta(r-b). \tag{2}$$

In this case, the corresponding potential in k-space can be obtained by the double (spherical) Bessel transform

$$V(k,k') = \int_0^\infty r^2 j_l(k'r)V(r)j_l(kr)\,\mathrm{d}r = \frac{\lambda b^2}{2\mu} j_l(k'b)j_l(kb). \tag{3}$$

The spherical Bessel function for $l=0$ is given by

$$j_0(z) = \frac{\sin(z)}{z}. \tag{4}$$

(a) Discretize the integral in Schrödinger's equation for N data points in a reasonable interval $[0, k_{\max}]$ using Gauss quadrature[1]. This will give you a linear eigenvalue problem of the form

$$\begin{pmatrix} H_{1,1} & H_{1,2} & \cdots \\ \vdots & \ddots & \\ H_{N,1} & & H_{N,N} \end{pmatrix} \cdot \begin{pmatrix} \psi_n(k_1) \\ \vdots \\ \psi_n(k_N) \end{pmatrix} = E_n \begin{pmatrix} \psi_n(k_1) \\ \vdots \\ \psi_n(k_N) \end{pmatrix}. \tag{5}$$

(b) Use a numerical library/program (e.g. LAPACK or the corresponding GSL variant, Mathematica, Matlab, Python) to find all eigenvalues of the above system. Identify the ground-state energy E_0 (has to be a bound state!). Use $l=0, \lambda=-10, \mu=1/2, b=5$ as initial parameters. Vary N and $k_{\max}$ to check whether your solution has converged.

(c) For $l=0$, the ground-state energy is determined by the transcendental equation

$$e^{-2\kappa b} - 1 = \frac{2\kappa}{\lambda}, \qquad E_0 = -\frac{\kappa^2}{2\mu}. \tag{6}$$

Solve this equation numerically and check your results against the solution.

[1] In Python, this can be done using the *numpy.polynomial.legendre.leggauss* function.

2. **Double Slits**

If you haven't finished it yet, implement the solution of the Schrödinger equation in two dimensions. Test your program with a Gaussian wave packet. As a reminder, the two-dimensional Schrödinger equation is

$$i\frac{\partial}{\partial t}\psi(\vec{\mathbf{r}},t) = -\frac{1}{2}\nabla^2\psi(\vec{\mathbf{r}},t) + V(\vec{\mathbf{r}},t)\psi(\vec{\mathbf{r}},t), \tag{7}$$

and the Gaussian wave packet can be written as

$$\psi(\vec{\mathbf{r}},t=0) = \exp\left(-\left(\frac{|\vec{\mathbf{r}}-\vec{\mathbf{r}}_0|^2}{2\sigma_0^2}\right)\right)\exp\Big(i\vec{\mathbf{k}}_0\cdot\vec{\mathbf{r}}\Big). \tag{8}$$

This time we want to study the behavior of a particle passing through a double-slit. Since fine-tuning the parameters of the problem can be time-consuming, we give you some advice:

- Choose a physical size of 10×10 in arbitrary units. A resolution of 128×128 points should be sufficient.
- You can model the slits with the same boundary condition you were using for the walls of the infinite square well. Put them at the center of the coordinate system.
- Put the initial wave packet one unit of length from the slits and give it a width of $\sigma_0 = 0.5$.
- Choose the wave vector $\vec{\mathbf{k}}_0$ so that it is perpendicular to the slit. What is the meaning of the length of $\vec{\mathbf{k}}_0$?

(a) Make plots of $|\psi|^2$ at different times. You can use the skeleton for solving the 2D Schrödinger equation of the last exercise.

(b) How does the interference pattern change when varying the wave number and slit size?

(c) Imagine the particle is detected on a screen at a certain distance from the slits. Plot the probability density on this screen. Compare it to the analytical expression

$$I(\sin(\theta)) = I(0)\cos^2\left(\frac{kD\sin(\theta)}{2}\right), \tag{9}$$

where I is the value of $|\psi|^2$ on the screen, D the distance between the slits, k the wave number, and θ the angle.

(d) When you have had enough fun with the double slits, you can change your program to calculate a single slit. Explore how the width of the slit and the wave number influence the picture on the screen.