

# 1 — PHY 494: Makeup assignment 1 (15 points total)

Due Thursday, April 22, 2021, 11:59pm.

This is a **optional Makeup Assignment**. If you choose to hand it in by the deadline, it will be graded like a normal homework assignment. If its grade is better than your worst homework grade then it will replace that grade.

Submission is to your **private GitHub repository**.

## 1.1 ODE with Scipy (15 points)

In this problem you should learn how to use existing functions in a library, namely in the `scipy` package (in particular, [scipy.integrate](#)). Part of the problem is to find and read the documentation for the function and figure out how to use it.

Use the Scipy function `scipy.integrate.solve_ivp()` to solve the following ordinary differential equation

$$-\frac{1}{2} \frac{d^2 \psi_n(x)}{dx^2} + \left[ \frac{1}{2} x^2 - E_n \right] \psi_n(x) = 0 \quad (1)$$

$$\psi_n(0) = 1; \quad \frac{d\psi_n(0)}{dx} = 0 \quad (2)$$

$$E_n = n + \frac{1}{2}, \quad n = 0, 2, 4, 6, \dots \quad (3)$$

for the real function  $\psi_n(x)$ <sup>1</sup> and the three values  $n = 0$ ,  $n = 2$ , and  $n = 8$ .

The code should contain the following functions:

1. **ode\_qmhosc()** solves the ODE Eq. 1:

```
psi = ode_qmhosc(x, psi0, dpsidx0, n=n)
```

that takes as arguments

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<sup>1</sup>If you have done Quantum Mechanics 1 (PHY 314) then you should recognize it as the Schrödinger equation for the simple harmonic oscillator.

- all the values  $x$  at which the solution should be evaluated (the first value *must* be the one for which the initial conditions are given, i.e.,  $x = 0$  for this problem),
- as initial conditions the function value and first derivative at  $x = 0$  (Eq. 2), and
- the value of  $n$  that determines  $E_n$  (Eq. 3).

It should return the function values  $\psi_n(x)$  as a numpy array.

2. `f_qmhosc()` is needed to transform the ODE Eq. 1 into standard form so that it can be solved with `scipy.integrate.solve_ivp()`.

`f_qmhosc(t, y, E)`

should produce the *ODE standard form*<sup>2</sup> of the derivative vector  $\mathbf{f}$  when provided with

- the current values of  $\mathbf{y}$
- the current value of  $t$
- and the parameter  $E_n$  (see Eq. 1).

The starter code in `makeup01.py` has additional hints on how to create a function that is suitable for `scipy.integrate.solve_ivp()`.

- (a) Numerically solve Eq. 1 on a lattice with  $\Delta x = 0.01$  for  $0 \leq x < 6$  for

- $n = 0$
- $n = 2$
- $n = 8$

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<sup>2</sup>Remember that the ODE standard form is

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}$$

and in the case of Eq. 1, we would have  $t = x$ ,  $y_0 = \psi_n(x)$ , and  $y_1 = \psi'_n(x) \equiv \frac{d\psi_n}{dx}$ .

Use the *rk45* solver (find out how to select it for the `solve_ivp()` function) and increase the default tolerance parameters for the solver to `rtol=1e-8, atol=1e-8`.

- (i) Write code that implements all the listed requirements. **[12 points]**
- (ii) Plot all your solutions in one figure and include the figure as a PDF named `qmhosc.pdf`. **[3 points]**

- (b) BONUS: Correct physical<sup>3</sup> solutions for Eq. 1 are *symmetric* ( $\psi(x) = \psi(-x)$ ) for even  $n$  and *antisymmetric* ( $\psi(x) = -\psi(-x)$ ) for odd  $n$ . This implies that the *initial conditions* for  $n = 1, 3, 5, \dots$  are different from the ones for even  $n$  (Eq. 2). Choose appropriate initial conditions<sup>4</sup> and write a function

```
phi0, dphidx0 = initial_values_qmhosc(n)
```

that produces the correct initial values depending on the value of  $n$ .

Using your initial values, solve Eq. 1 for  $n = 3$  and plot the solution (include a PDF named `qmhosc_odd.pdf`). **[bonus +4\*]**

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<sup>3</sup>Physical solutions for the wavefunction  $\psi_n(x)$  have to be normalizable, i.e., they have to decay to zero for  $x \rightarrow \pm\infty$ . The numerical solutions only fulfill this requirement for small  $x$  and even for moderately large  $x$  they start to diverge. It would be better to use specialized algorithms that have the normalizability requirement built in.

<sup>4</sup>Choose  $\psi(0) \geq 0$ ,  $\frac{d\psi(0)}{dx} \geq 0$  and either use values of 0 or 1 because this is the convention employed in the tests.