Assignment 5B

- **Problem 1 (100 points): Anharmonic Oscillator**

Consider the Schrödinger equation for a particle of mass m in the anharmonic potential $V(x) = V_0 \frac{x^4}{a^4}$:

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{1}$$

where V_0 and a are constants. For simplicity, in this exercise set $\frac{V_0}{a^4} = \frac{1}{2}$.

After converting this second-order equation into a 2-dimensional first-order equation, write a program to solve this system using the shooting method and the 4th-order Runge-Kutta (RK4) method.

As explained in class, you will need to write a program to find the energies, starting with an initial guess for the energy and using a root-finding method to refine the guess until you find accurate values.

Note that, as opposed to the harmonic oscillator, there is no exact analytical solution (at least, not for all eigenstates).

Important Trick 1 (Solving the system in a "large box"): Note that, in theory, the wavefunction is non-zero for any finite value of x, as it is required to vanish only in the limit for $x = \pm\infty$. But you can obtain good approximate solutions by using a large but finite interval.

Hint: For the chosen parameters, setting the box of size $[-N, N]$ with $N = 4$ leads to sufficient accuracy

Important Trick 2 (Using the WKB formula to guide the numerical search for the energy eigenvalues): To guide your initial energy guesses for the root-finding method, use the WKB formula derived in class.

(a) **(30 points)** Use Simpson's method to calculate the relevant numerical integral in the WKB formula:

$$B = \int_{-1}^{1} ds\,\sqrt{1 - s^4}$$

and obtain the corresponding WKB approximations to the eigenvalues:

$$E_n \sim \frac{1}{2}\left(\pi \frac{n + \frac{1}{2}}{\int_{-1}^{1} ds\,\sqrt{1 - s^4}}\right)^{\frac{4}{3}} \qquad n = 0, 1, 2, \ldots . \tag{2}$$

Hint: Note that the integrand of B is relatively steep near the integration boundaries. Make sure to use a sufficiently tight mesh to have at least 4 significant digits of accuracy in the eigenvalues, for $n = 0, 1, ..., 6$.

(b) **(50 points)** Start from one of the boundaries —in a similar fashion as in the example of the infinite square well discussed in class.

Calculate the eigenfunctions and the eigenvalues of the problem for $n = 0, 1, ..., 6$ (for simplicity, you are not required to normalize the wavefunctions in this exercise).

(c) **(20 points)** Compare your numerical energy eigenvalues with the WKB energies and plot the results as a function of the excitation number n. Discuss the agreement as a function of n.