Exercise Sheet 3

1. *matching*

Calculate the radial wave function on a radial grid by integrating outwards $v_i^{\rightarrow}$ and inwards $v_i^{\leftarrow}$ on the logarithmic grid to the matching point x_M.

i. Find the classical turning points on the logarithmic grid. How many are there for any given l?

ii. Consider the radial function obtained by putting together the two solutions at the matching point

$$v_i = \begin{cases} v_i^{\rightarrow}\, v_M^{\leftarrow} & \text{for } i \leq M \\ v_i^{\leftarrow}\, v_M^{\rightarrow} & \text{for } i \geq M \end{cases}$$

Normalize v on the logarithmic grid using

$$\int_0^{\infty} dr\, |u(r)|^2 = \int_{-\infty}^{\infty} dx\, r^2\, |v(x)|^2$$

Estimate the contributions from the missing regions $x < x_{\text{min}}$ and $x > x_{\text{max}}$.

iii. By what Δk_M^2 would you have to change the original k_M^2 so that v_i is a solution of the radial eigenvalue problem? Hint: look at the Numerov iteration connecting v_{M-1}, v_M, and v_{M+1} and solve for k_M^2, assuming $k_{M\pm1}^2$ are unchanged.

iv. When considering $-\Delta k_M^2$ as perturbation to the above exact solution, we can estimate the eigenenergy for the potential we are interested in using first-order perturbation theory.

v. For the integration at the new energy use the normalization factor for getting reasonable values for initializing the wave functions.

vi. Stop when the change in energy is smaller than the desired accuracy.