Exercise Sheet 3 due 30 April 2018

1. *matching*

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

i. Write a routine to find the classical turning points on the logarithmic mesh. How many are there for any given l?

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

$$\tilde{u}_i = \begin{cases} \tilde{u}_i^{\rightarrow}\, \tilde{u}_M^{\leftarrow} & \text{for } i \leq M \\ \tilde{u}_i^{\leftarrow}\, \tilde{u}_M^{\rightarrow} & \text{for } i \geq M \end{cases}$$

Normalize $\tilde{u}$ on the logarithmic mesh using

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

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

iii. By what Δk_M^2 would you have to change the original k_M^2 so that $\tilde{u}_i$ is a solution of the radial eigenvalue problem? Hint: look at the Numerov iteration connecting $\tilde{u}_{M-1}$, $\tilde{u}_M$, and $\tilde{u}_{M+1}$ 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.