PHY 304, II-Semester 2021/22, Assignment 4

Instructor: Sebastian Wüster
Due-date: 17. March. 2024, Note long deadline due to dead week and midsem break. If you do not want to spoilt your mid-sem break, feel free to hand in by 10th March instead.

(1) Variational Hydrogen atom: [8 pts] Apply the variational method to the Hydrogen atom, with the Hamiltonian from Eq. (4.72) QM-I ($\hat{H}_{rel}$ only).

(a) Use the trial wavefunction $\phi(\mathbf{r}) = \mathcal{N} e^{-\beta r^2}$, with $r = \sqrt{x^2+y^2+z^2}$, to find an approximation for the ground-state energy and ground-state wavefunction [3pts]

(b) Do the same, using the trial wavefunction $\phi(\mathbf{r}) = \mathcal{N} e^{-\alpha r}$ instead. [3pt]

(c) Compare both results for wavefunction and energy with the known true solution and discuss. [2pts]

(2) Negative Hydrogen ion: [6 pts] In the lecture we discussed the application of a variational Ansatz, Eq. (7.101) to approximate the ground-state of Helium, in which two electrons are bound to the Helium nucleus through the Coulomb potential. Instead we could attempt the same Ansatz and calculation for two electrons attached to a single proton, which would form H^-, a negatively charged Hydrogen ion.

(a) Do that for the same trial wavefunction that we had used for Helium in the lecture and discuss the implications of your result for the ground-state energy [2pts].

(b) Now do the same for the more sophisticated two-electron trial wavefunction

$$\psi(\mathbf{r}_1,\mathbf{r}_2) = \mathcal{N}\left[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) + \phi_2(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\right], \qquad \text{with}$$
$$\phi_1(\mathbf{r}) = \sqrt{\frac{Z_1^3}{\pi a_0^3}} e^{-Z_1 r}, \qquad \phi_2(\mathbf{r}) = \sqrt{\frac{Z_2^3}{\pi a_0^3}} e^{-Z_2 r}, \tag{1}$$

for $Z_1, Z_2 > 0$ real and adjustable, a_0 the Bohr radius, and $\mathcal{N}$ a normalisation factor. Which ground state energy do you find now, how does this change your conclusions and what would have to be the spin state of the two electrons? [4pts].

(3) WKB approximation: [8 pts] Using the WKB method, calculate the transmission coefficient for the potential barrier ($V_0, a > 0$)

$$V(x) = \begin{cases} V_0\left(1 - \frac{|x|}{a}\right) & \text{if } |x| \le a \\ 0 & \text{if } |x| > a, \end{cases} \tag{2}$$

for all values of E.

(4) WKB approximation in complex potential landscape: [**8 pts**] The matlab script `Assignment4_program_draft_v3.nb` solves the TISE numerically as seen in e.g. Assignment 3 QM-I for the exact same potential as the movie frames in Example 1 QM-1. Run the script once, to generate the eigenstates and energies.

(a) By changing `statepick` you can choose which eigenvector is shown (in the usual style where we change the baseline of the eigenfunction to sit on the energy). Make a few plots of qualitatively different states, and discuss, based on your insight of the WKB approximation, why they take the form shown. In particular focus on the states where the eigenenergy is close to (below and above) that local maximum (hump) in the potential. [3pts] *Note that solutions must use the mathematica code and plotting tools.*

(b) Now upgrade `Assignment4_program_draft_v3.nb` at the bottom such that it can also calculate, tabulate, and plot the WKB approximation of the eigenstates that you implement, based on the classical momentum $p(x)$ and the energy E_n (taken as known, from the numerical solution of the TISE). Plot those directly on top of the numerically found states, and discuss for a few examples. Plot the true and the WKB solution for a couple of cases where it works well or not so well, and discuss why either is the case. [5pts]