PHY 304, II-Semester 2023/24, Tutorial 4

22. Feb 2024

Work in the same teams as for assignments. Do "Stages" in the order below.
Discuss on your table. When all teams finished a stage, make sure all students at your table understand the solution and agree on one by using the board.

Stage 1 Variational method for atomic and molecular physics:

(a) Discuss why (or under which conditions) the variational wavefunction:

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \frac{Z_{\text{eff}}^3}{\pi a_0^3} e^{-Z_{\text{eff}}(r_1+r_2)/a_0}, \tag{1}$$

could be a good Ansatz for the Helium Hamiltonian.

$$\hat{H} = -\frac{\hbar^2}{2m_e}\left(\Delta_{\mathbf{r}_1} + \Delta_{\mathbf{r}_2}\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right). \tag{2}$$

(see section 7.5.1)

(b) Propose at least one wavefunction that adds an extra parameter to variationally take into account electron-electron repulsion.

(c) Discuss why (or under which conditions) the variational wavefunction:

$$\psi_0(\mathbf{r}) = \frac{\mathcal{N}}{\sqrt{2}}\left(\phi_{100}(\mathbf{r}) + \phi_{100}(\mathbf{r}')\right) = \frac{\mathcal{N}}{\sqrt{2\pi a_0^3}}\left(e^{-r/a_0} + e^{-r'/a_0}\right), \tag{3}$$

could be a good Ansatz for the H_2^+ Hamiltonian.

$$\hat{H} = -\frac{\hbar^2}{2m_e}\Delta_{\mathbf{r}} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r} + \frac{1}{r'} - \frac{1}{R}\right). \tag{4}$$

(see section 7.5.2)

(d) Using this, what is the essence of a covalent molecular bond that we discover?

(e) Propose one or two physically motivated ways how the Ansatz (3) could be made more powerful by introducing variational parameters.

Stage 2 WKB approximation

(i) Discuss in your team what constitutes the WKB approximation, what is the basic idea, and how one can estimate whether it will be valid.

(ii) Based on your summary, inspect Fig. 1 below and discuss for each case whether WKB will be good and why, where it won't be good or why it won't be good.

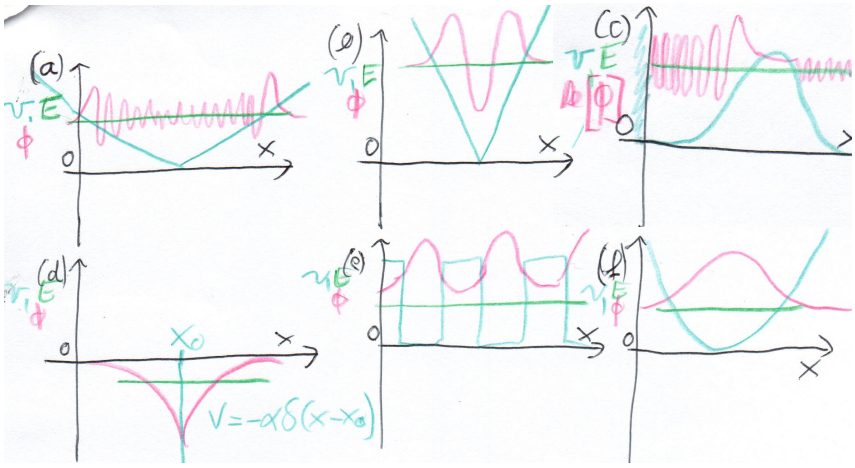

Figure 1: (**stage 2**) Potentials $V(x)$ (cyan) and energies E (green) are drawn on the same scale. Wavefunctions $\phi(x)$ are arbitrarily scaled and drawn with $\phi = 0$ on the green line (except in [d], where $\phi = 0$ is the black line).

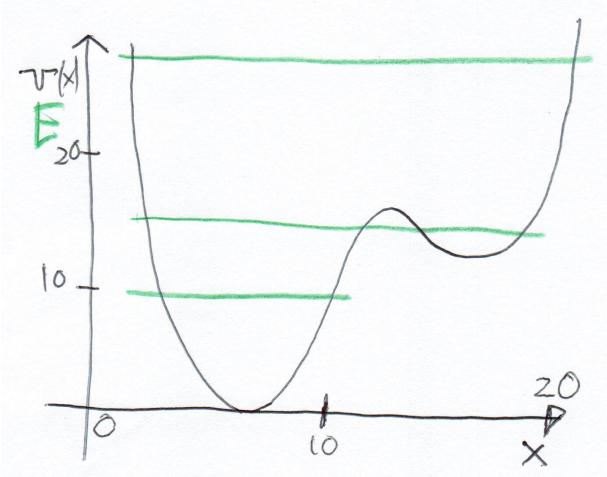

Figure 2: (**stage 2**) Potential for Stage 2 (iii).

(iii) In Fig. 2, draw your own guess at the WKB wavefunction for the energies indicated, and discuss within your team. Take into account the given values for V, E (dimensionless units) and assume $h = 1$ and importantly a mass $m = 1/320$.

(iv) With drawings and discussions, elaborate on how one arrives at the WKB connection formula Eq. (7.139) and what its uses are.