PHY453 Computational Physics | Assignment 7

Anantha Rao | Reg no: 20181044

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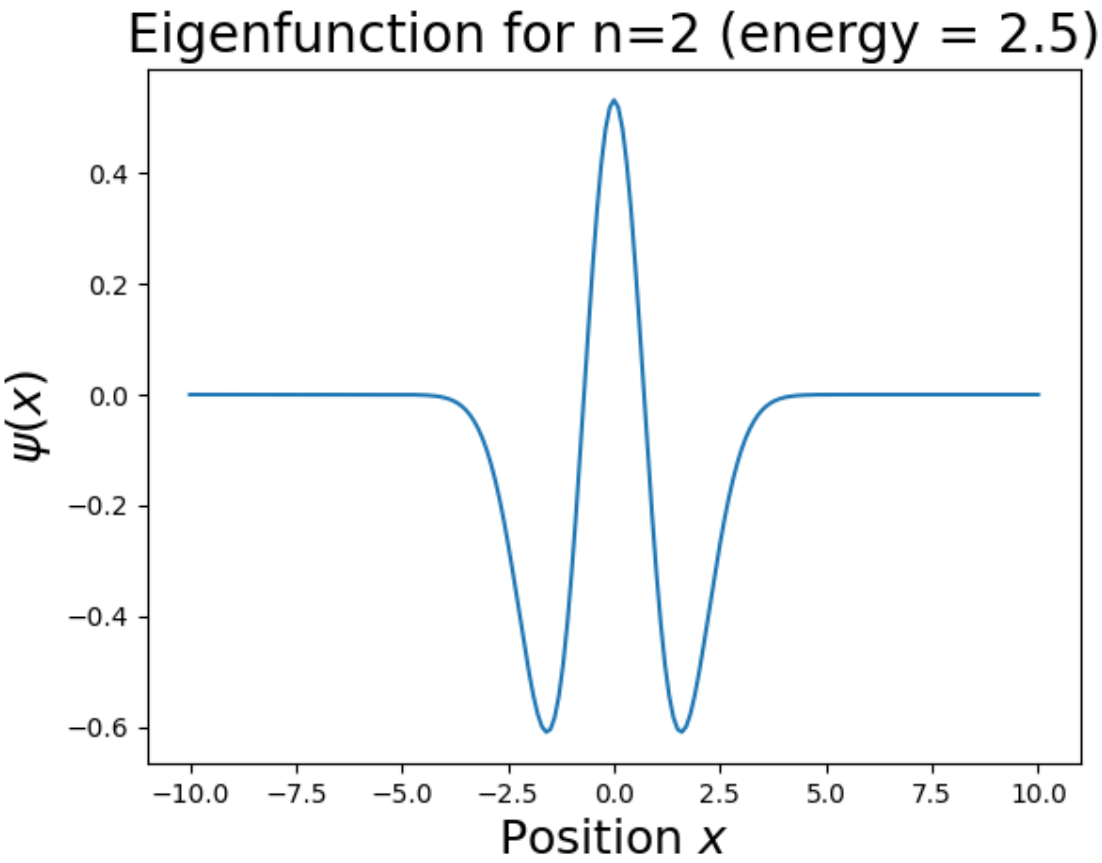
Q1.



(a) The eigenvalue for the n=2 state is 2.5 units

(b) The accuracy of the result is given by the threshold we set in the program. Here we have used a threshold (ε) = 1e-10

(c) On varying the mesh size, we see that the wavefunction smoothens out. As we increase the mesh size, the first derivative's discontinuity at the maxima and the minima's tends to vanish. This occurs due to the smaller dx values from increasing the mesh-size. The eigenvalue increases to larger than 2.5 if we increase x_max and keep the grid points constant. On varying x_max, the wavefunction's width varies. When we increase x_max, the first derivative's discontinuity increases and becomes more prominent. Reducing the x_max gives us smaller values of dx, thus making the test-space more quasi-continuous. I think that increasing x_max while keeping the number of grid points constant decreases the accuracy of the approximation, we use but when we keep x_max fixed and increase grid points then we increase the accuracy since we're taking finer divisions.

Q2. (a) For V=1, b=2, the first three energy eigenvalues are: (-0.521007, 1.191738, 1.240160)

- The first eigenvalue corresponds to the single bound state (ground state) for the system whereas the other two smallest eigenvalues represent the first scattering states. These values change when the parameters (a: periodicity, n: no of plane waves) are modified.
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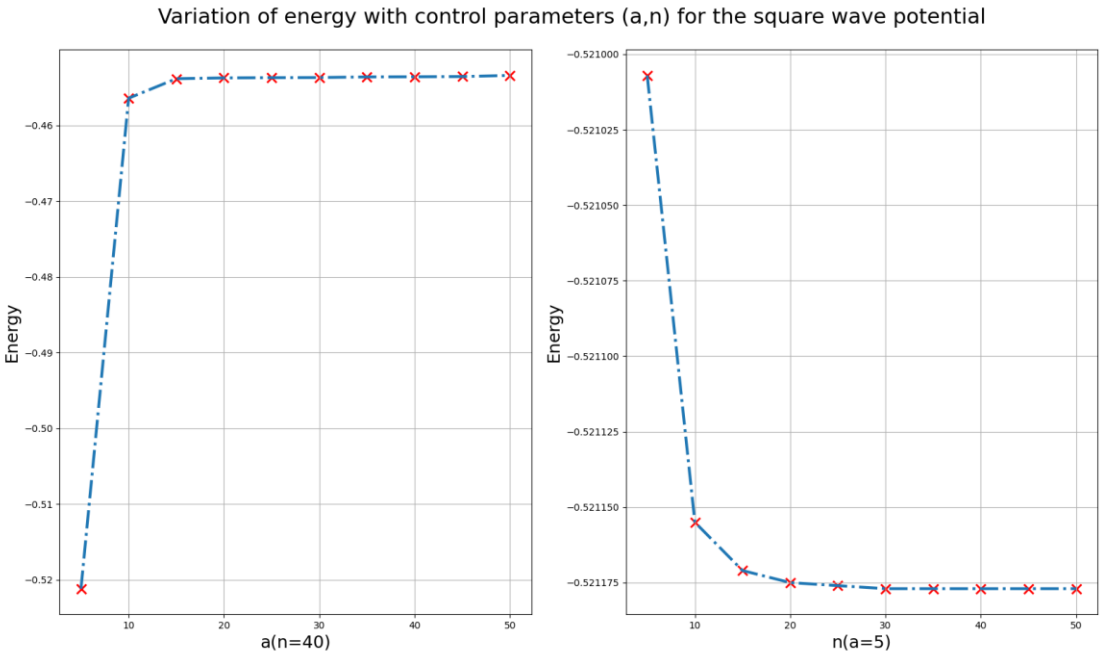

Physical interpreation:

(b) **Effect of changing 'a' on energy (au)**:

The parameter 'a' is used as a measure of distance between neighbouring potential wells when we consider perioidic boundry conditions (PBC). For small 'a' values, successive wells are strongly coupled and this leads to reduced overall energy of the system (as seen in the above figure). When the periodicity of the plane waves increases, aliter, when 'a' is infinitely large, only then do we simulate the actual well. As we increase the value of 'a', the periodic potentials move farther away, interact less, the energy of the system increases, and this signals that the interaction between successive attractive square well potentials decreases. We notice that after a > 15, the energy of the system remains constant. Hence a=15 can be chosen to be a suitable value for PBC.

(c) **Effect of changing 'n' on energy:**

The parameter 'n' represents the number of plane waves used or the size of the basis set used for the simulation. As 'n' increases, energy goes down and gradually converges to a particular value. From the variational principle, we know that, the higher the number of wave functions we use in the expansion of unknown wave function, the closer we approach the ground state of the system. Since the value of energy obtained from this method is always higher than the actual ground state of the system, when we increase the size of the basis, we approach the ground state energy from the right. From the figure n=30, seems to be an ideal size to achive convergence.