

Variational Principle Assignment

Due date: 27/03/2023

1) Using the variational principle and plane wave basis, determine the eigenvalues for the following square well potential: (10 marks)

$$V(x) = 0 \text{ for } x > b/2 \text{ and } x < -b/2$$

$$V(x) = -V \text{ for } -b/2 \leq x \leq b/2$$

Assume the plane waves have a periodicity a ; $a > b$.

Use atomic units. Requires lapack dsyev

Answer the following questions:

(a) For $V=1$, $b=2$ what is the energy?

(b) Plot the energy as a function of ' a '. Explain what you observe.

(c) Plot the energy as a function of no. of plane waves. What do you observe? Explain your observation.