- 1) Using the Numerov method determine the solutions for the quantum mechanical harmonic oscillator (use adimensional units). Use xmax=10 and 100 grid points. Answer the following questions: (10 marks)
- (a) Plot the eigenfunction for n=2. What is the corresponding eigenvalue you obtain?
- (b) How accurate are your results?
- (c) How do the results (eigenfunctions and eigenvalues) change if you reduce xmax keeping the grid points same and vice versa? Explain your observation.
- 2) Using the variational principle and plane wave basis, determine the eigenvalues for the following square well potential: (10 marks)

$$V(x) = 0$$
 for  $x > b/2$  and  $x < -b/2$ 

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

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.