```
> restart;
```

Solve for the energies of the square wave potential. Work the problem in units

where hbar/2m=a=1.

```
> Digits:=10;
```

$$Digits := 10$$

Need the linalg package to get the "eigenvectors" function.

```
> with(linalg):
```

```
Warning, the protected names norm and trace have been redefined and
unprotected
```

Define the matrix from the Central Equation derived for the square wave potential. Udc is the zero frequency component of U (the average potential).

```
> M:=<<Udc+(k-2*2*Pi)^2,1/Pi,0,-1/(3*Pi),0>|
                  <1/Pi,Udc+(k-1*2*Pi)^2,1/Pi,0,-1/(3*Pi)>|
            <0,1/Pi,Udc+k^2,1/Pi,0>|
            <-3/Pi,0,1/Pi,Udc+(k+1*2*Pi)^2,1/Pi>|
            <0,-3/Pi,0,1/Pi,Udc+(k+2*2*Pi)^2>>;
```

```
>
```

$$M := \begin{bmatrix} Udc + (k - 4\pi)^2 & \frac{1}{\pi} & 0 & -\frac{3}{\pi} & 0 \\ \frac{1}{\pi} & Udc + (k - 2\pi)^2 & \frac{1}{\pi} & 0 & -\frac{3}{\pi} \\ 0 & \frac{1}{\pi} & Udc + k^2 & \frac{1}{\pi} & 0 \\ -\frac{1}{3\pi} & 0 & \frac{1}{\pi} & Udc + (k + 2\pi)^2 & \frac{1}{\pi} \\ 0 & -\frac{1}{3\pi} & 0 & \frac{1}{\pi} & Udc + (k + 4\pi)^2 \end{bmatrix}$$

Set Umax equal to 1 which means Udc=0.5.

```
> M;
```

$$\begin{bmatrix} Udc + (k - 4\pi)^2 & \frac{1}{\pi} & 0 & -\frac{3}{\pi} & 0 \\ \frac{1}{\pi} & Udc + (k - 2\pi)^2 & \frac{1}{\pi} & 0 & -\frac{3}{\pi} \\ 0 & \frac{1}{\pi} & Udc + k^2 & \frac{1}{\pi} & 0 \\ -\frac{1}{3\pi} & 0 & \frac{1}{\pi} & Udc + (k + 2\pi)^2 & \frac{1}{\pi} \\ 0 & -\frac{1}{3\pi} & 0 & \frac{1}{\pi} & Udc + (k + 4\pi)^2 \end{bmatrix}$$

```
> Udc:=0.5;
```

$$Udc := 0.5$$

Pick one k value to find energies and corresponding eigenfunctions.

```
> k:=Pi;
```

$$k := \pi$$

```
> ;
```

```
> Eigs:=eigenvectors(M);
```

```
Eigs := [89.64569522, 1,
        {[0.9491328356, 0.003798210201, -0.001253761366, -0.3160514718, 0.0006409193547]}],
        [89.00910918, 1,
        {[1.580026464, 0.006417056967, 0.002159902560, 0.5271939787, -0.001056241719]}], [10.04981412,
        1, {[-0.002803352425, 0.7066804287, -0.7062267261, 0.0028306213, 0.0003123236681]}],
        [10.68640017, 1,
        {[-0.002899134028, 0.7076310135, 0.7081278815, -0.0028714884, 0.0003212633841]}], [
        247.2411797, 1,
        {[0.00002031646619, 0.004031643110, 0.0000027086, -0.00201580933, -1.000046810]}]
```

The above is a list of five entries for the five energy eigenvalues and eigenvectors.

The first entry in each list item is then energy eigenvalue.

The next entry is the degeneracy. All our eigenvectors are non-degenerate.

The next entry is the eigenvector, telling us how much (C_i) of the each of the five psi(k+G) basis functions.

We need to build a sum of C_i * Psi_i over the five wave functions.

Here, recall that adding a subscript "[3]" to a list pulls out the third item in the list. For example, to get the fourth component of the second eigenvector, we would have a sequence

[2] -- second eigenvector

[3] -- the third entry in this eigenvector entry, which is the set of one eigenvector in the entry.

[1] -- selects the first and only eigenvector in this list. (This just strips off the curly brackets from the eigenvector.)

[4] -- selects the fouth component of this vector.

For example:

```
> psi:=Eigs[2][3][1][4]*exp(I*(k-2*Pi)*x);
```

$$\psi := 0.0028306213\, e^{(-I\,\pi\,x)}$$

Now construct our G=2 pi j/a sum, h=-2..2. Note that j=-2 is eigenvector 1, so I need to add 3 to convert j to a subscript.

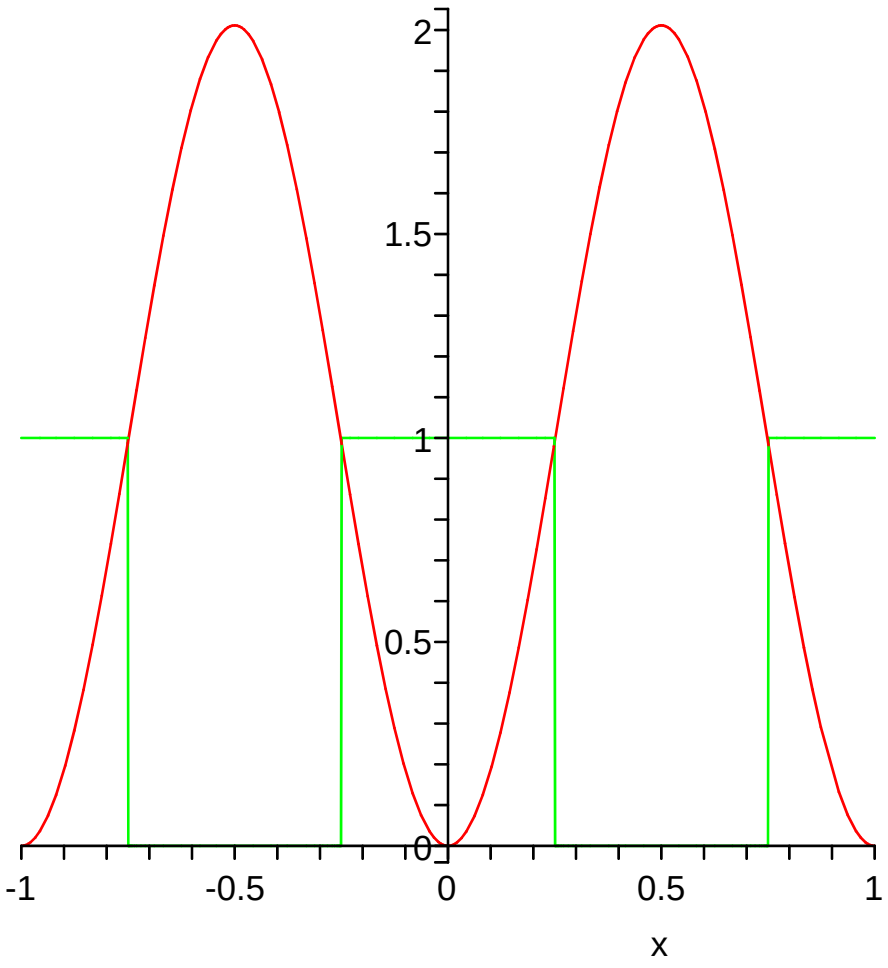
Let's do it first for the ground state, the third eigenvalue/eigenvector.

```
> psi2:=sum(Eigs[3][3][1][j+3]*exp(I*(k-j*2*Pi)*x),j=-2..2);
```

$$\psi 2 := -0.002803352425\, e^{(5\,I\,\pi\,x)} + 0.7066804287\, e^{(3\,I\,\pi\,x)} - 0.7062267261\, e^{(I\,\pi\,x)} + 0.0028306213\, e^{(-I\,\pi\,x)} + 0.0003123236681\, e^{(-3\,I\,\pi\,x)}$$

Now plot the result, along with the potential. Note that Heaviside(cos) gives me the desired square potential.

```
> plot({Heaviside(cos(2*Pi*x)),conjugate(psi2)*psi2},x=-1..1);
```



We can see why it is a low energy state. The charge is fairly uniform, but preferentially piled up in the

potential wells.

(Ignore the average height. The wave function is not normalized.

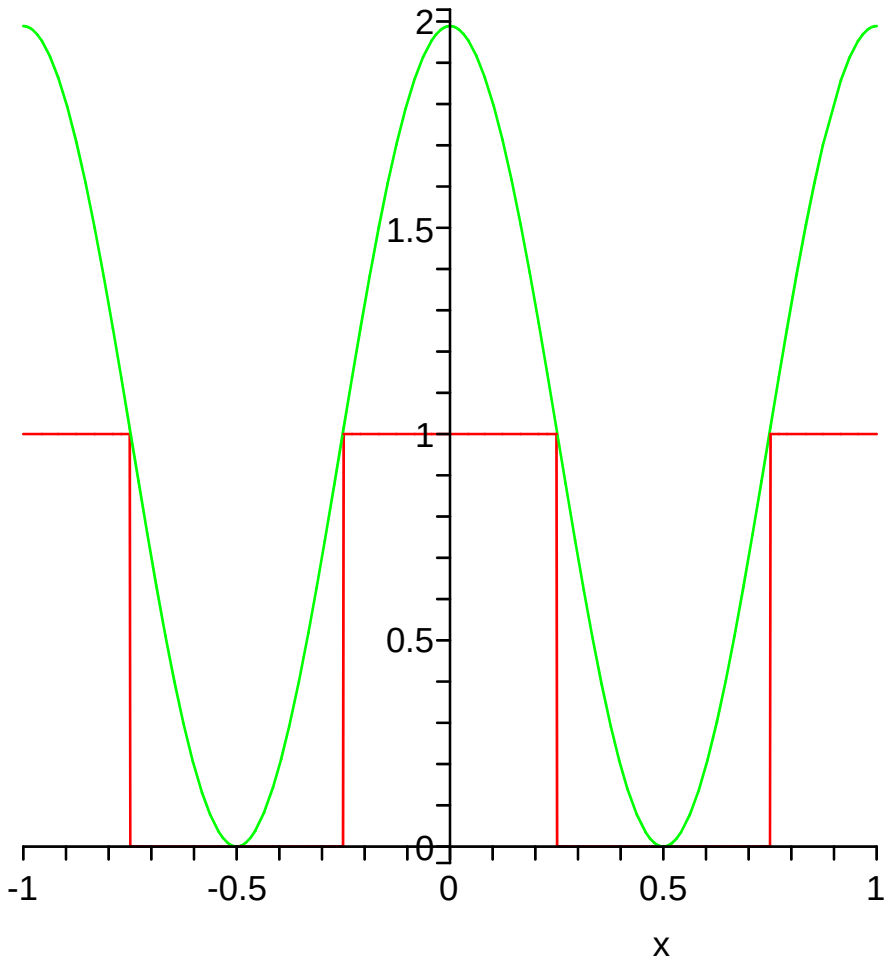
Now let's look at second lowest state, the fourth eigenvector.

```
> psi2:=sum(Eigs[4][3][1][j+3]*exp(I*(k-j*2*Pi)*x),j=-2..2);
```

$$\psi 2 := -0.002899134028\, e^{(5\, I\, \pi\, x)} + 0.7076310135\, e^{(3\, I\, \pi\, x)} + 0.7081278815\, e^{(I\, \pi\, x)} - 0.0028714884\, e^{(-I\, \pi\, x)} + 0.0003212633841\, e^{(-3\, I\, \pi\, x)}$$

Now plot the result, along with the potential. Note that Heaviside(cos) gives me the desired square potential.

```
> plot({Heaviside(cos(2*Pi*x)),conjugate(psi2)*psi2},x=-1..1);
```



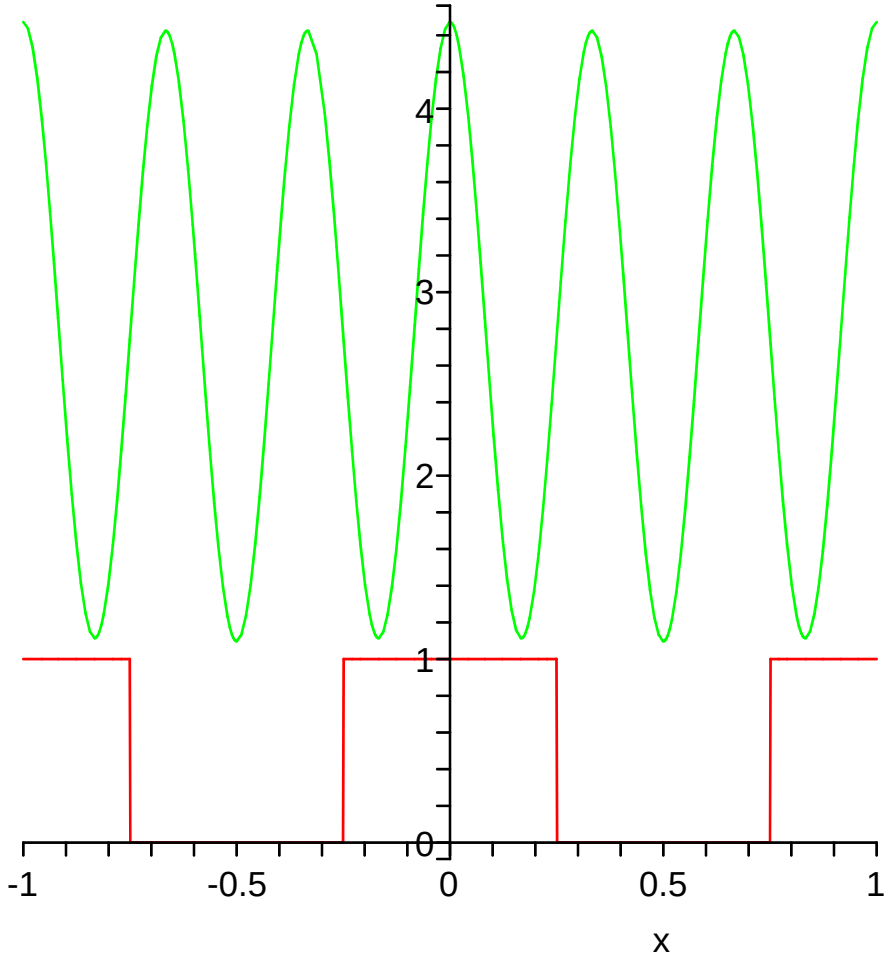
We can see why this is higher potential energy.

Let's look at the third level, eigenvector 2:

```
> psi2:=sum(Eigs[2][3][1][j+3]*exp(I*(k-j*2*Pi)*x),j=-2..2);
```

$$\psi 2 := 1.580026464\, e^{(5\, I\, \pi\, x)} + 0.006417056967\, e^{(3\, I\, \pi\, x)} + 0.002159902560\, e^{(I\, \pi\, x)} + 0.5271939787\, e^{(-I\, \pi\, x)} - 0.001056241719\, e^{(-3\, I\, \pi\, x)}$$

```
> plot({Heaviside(cos(2*Pi*x)),conjugate(psi2)*psi2},x=-1..1);
```




```
>
```

Lower potential and much higher kinetic energy.