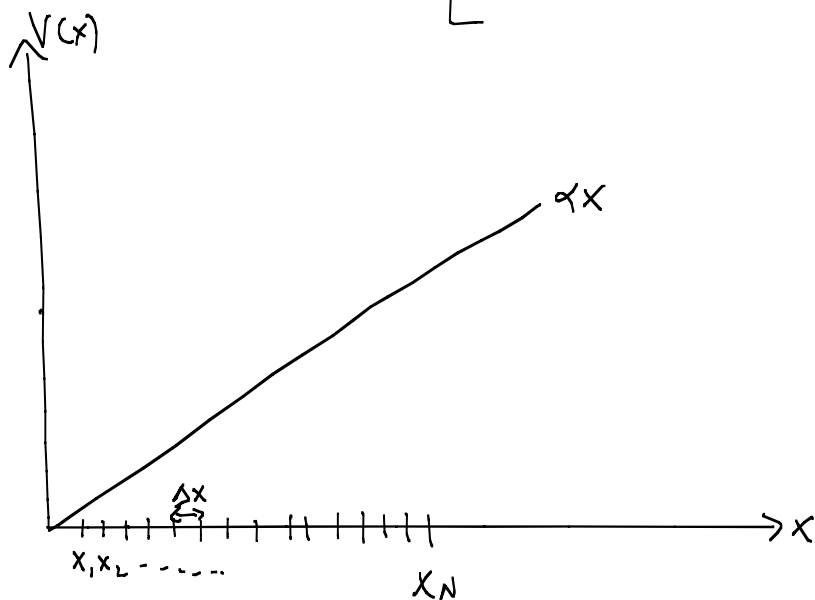


2.

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi = E \psi$$



$$\begin{bmatrix} \frac{\hbar^2}{m\Delta x^2} + V(x_1) & -\frac{\hbar^2}{2m\Delta x^2} & 0 & 0 & \dots \\ -\frac{\hbar^2}{2m\Delta x^2} & \frac{\hbar^2}{m\Delta x^2} + V(x_2) & -\frac{\hbar^2}{2m\Delta x^2} & 0 & \\ & & & \ddots & \\ & & & & \ddots \end{bmatrix} \begin{bmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_N) \end{bmatrix} = E \begin{bmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_N) \end{bmatrix}$$

```
clear
close all;
```

```
c=2.998e10;%cm/s
hbar=6.582e-16;%in eV*sec
m=5.11e5/c^2;%in eV/c^2
```

```
dx=1e-9;%0.1 Ang, in cm
tx=hbar^2/(2*m*dx^2);
```

```
N=100;%size of matrix
```

```
x=dx*(1:N);
V=1e9*x;%half-triangle potential
```

```
H=tx*(diag(2*ones(N,1))+diag(-1*ones(N-1,1),1)+diag(-1
*ones(N-1,1),-1))+diag(V);
```

```
[v,d]=eig(H);
```

```
psi1=v(:,1);
psi2=v(:,2);
psi3=v(:,3);
```

plot

```
figure(1);
plot(x*1e7,V,'k;potential V(x);')
xlabel('distance [nm]');
ylabel('potential energy [eV]')
title('Half-triangular well: \alpha=10^9 eV/cm')
```

```
figure(2)
plot(x*1e7, conj(psi1).*psi1,'k;1st;')
hold on
plot(x*1e7, conj(psi2).*psi2,'r;2nd;')
plot(x*1e7, conj(psi3).*psi3,'b;3rd;')
hold off
```

plot

```
title('Half-triangular well, \alpha=10^9 eV/cm: electron density distributions')
xlabel('distance [nm]');
ylabel('\Psi * \Psi')
```

```
figure(3)
plot(diag(d),'*');
xlabel('quantum number n')
ylabel('Energy eigenvalue [eV]')
title('Half-triangular well, \alpha=10^9 eV/cm: energy eigenvalues')
axis([0 10 0 100])
```

```
expct_x=psi1'*diag(x)*psi1;
```

<x>: expct_xsqrd=psi1'*diag(x.^2)*psi1;

<x^2>: Dx=sqrt(expct_xsqrd-expct_x^2);

Δx :

$\frac{h}{4\pi}$: p=hbar/i*(diag(ones(length(psi1)-1,1),1)+diag(-ones(length(psi1)-1,1),-1))/(2*dx);
 $\frac{h^2}{8m}$: psqrd=-hbar^2*(diag(-2*ones(length(psi1),1))+diag(ones(length(psi1)-1,1), 1)+diag(ones
(length(psi1)-1,1), -1))/dx^2;

```
expct_p=psi1'*p*psi1;
```

<p>:

```
expct_psqrd=psi1'*psqrd*psi1;
```

<p^2>:

```
Dp=sqrt(expct_psqrd-expct_p^2);
```

Δp :

```
disp(['<x>=' num2str(expct_x*1e7) ' nm'])
```

```
disp(['<x^2>=' num2str(expct_xsqrd*1e14) ' nm^2'])
```

```
disp(['<p>=' num2str(expct_p*1e-7) ' nm^-1'])
```

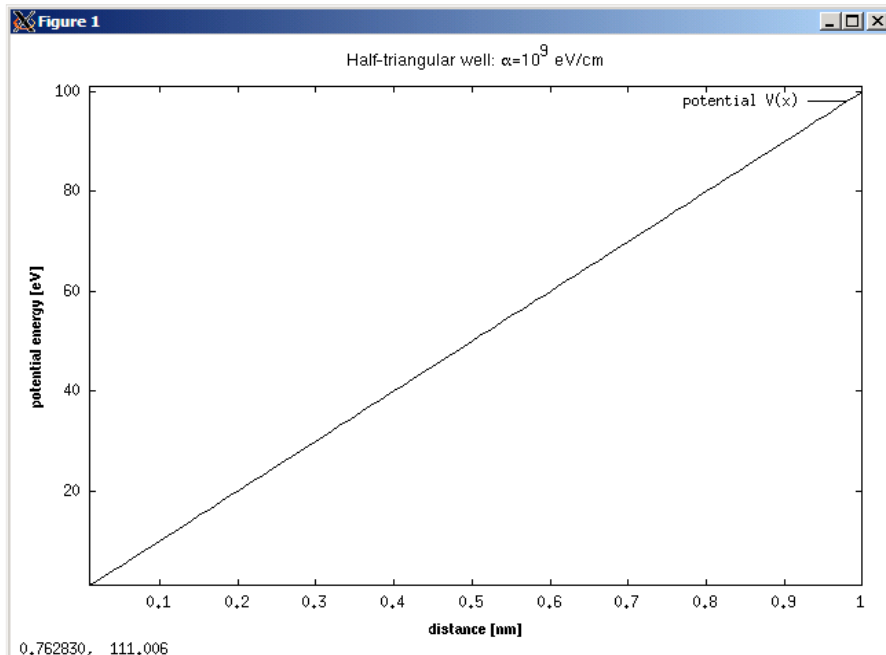
```
disp(['<p^2>=' num2str(expct_psqrd*1e-14) ' nm^-2'])
```

```
disp(['Delta_x=' num2str(Dx*1e7) ' nm'])
```

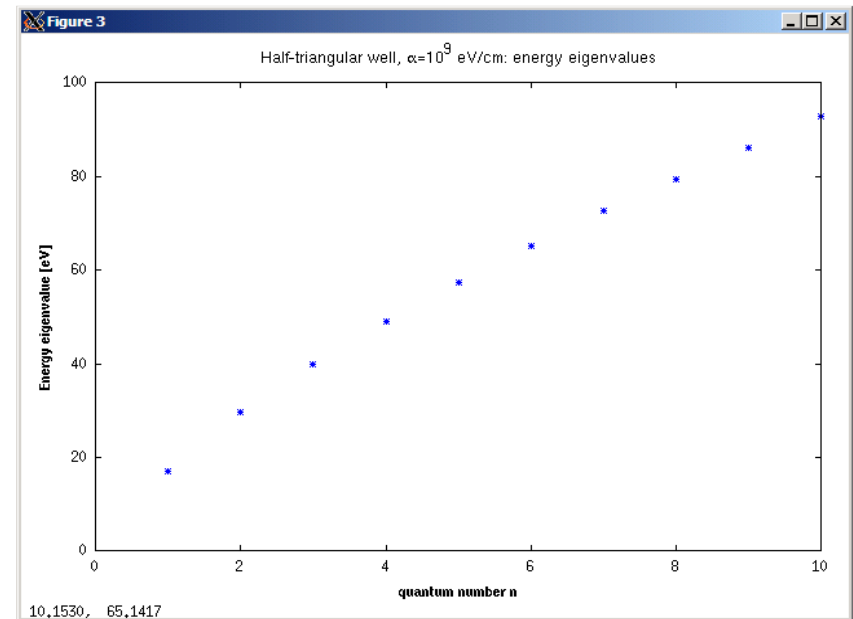
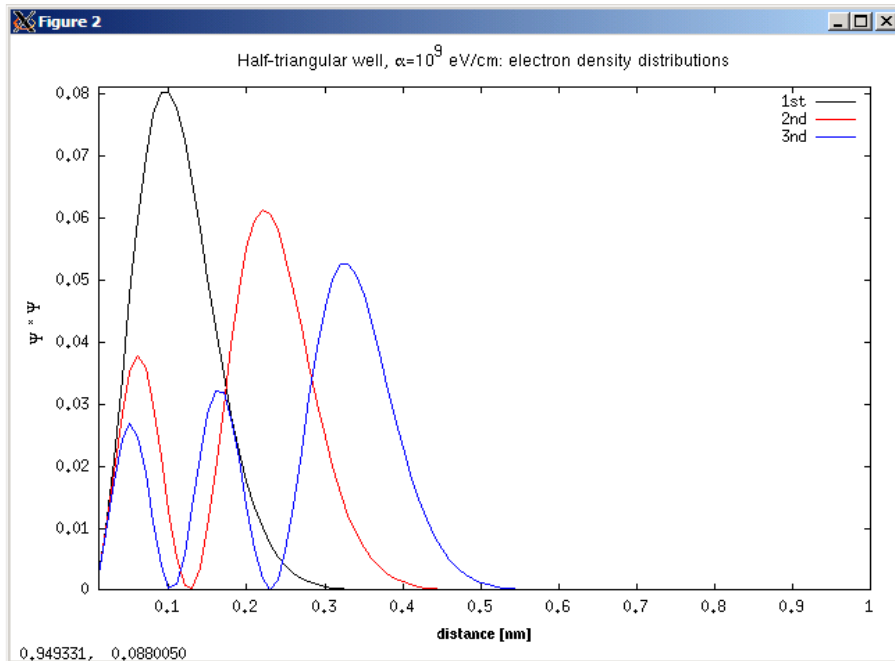
```
disp(['Delta_p=' num2str(Dp*1e-7) ' nm^-1'])
```

```
disp(['Heisenberg: Dx*Dp (in units of hbar/2):' num2str(2*Dx*Dp/hbar) ' (should be > 1)']);
```

$$\Delta x \Delta p \geq \frac{h}{2}$$



```
octave:1> triangleSE
<x>=0.11283 nm
<x^2>=0.015281 nm^2
<p>=0-1.3566e-31i nm^-1 ← ≈ 0
<p^2>=6.4293e-29 nm^-2
Delta_x=0.050496 nm
Delta_p=8.0183e-15 nm^-1
Heisenberg: Dx*Dp (in units of hbar/2):1.2303 (should be > 1)
```



$$2. \text{ i) } \int_{-\infty}^{\infty} \Psi^* \Psi dx = \int_0^a A^2 (\cancel{\Psi_1^* \Psi_1^1} + \cancel{\Psi_2^* \Psi_2^1} + \cancel{\Psi_1^* \Psi_2^0} + \cancel{\Psi_2^* \Psi_1^0}) dx$$

$$= A^2 \cdot 2 = 1 \quad A = \sqrt{\frac{1}{2}}$$

Ψ_n 's are orthonormal

$$\text{ii) } \Psi(x, t) = \frac{1}{\sqrt{2}} \left(\Psi_1(x) e^{-i \frac{E_1}{\hbar} t} + \Psi_2(x) e^{-i \frac{E_2}{\hbar} t} \right)$$

$$|\Psi(x, t)|^2 = \Psi^*(x, t) \Psi(x, t)$$

$$= \frac{1}{2} \left[\Psi_1^*(x) \Psi_1(x) + \Psi_2^* \Psi_2 + \Psi_1^* \Psi_2 e^{i \left(\frac{E_1 - E_2}{\hbar} \right) t} + \Psi_2^* \Psi_1 e^{-i \left(\frac{E_1 - E_2}{\hbar} \right) t} \right]$$

$$= \frac{1}{2} \left[\Psi_1^2(x) + \Psi_2^2(x) + 2 \Psi_1(x) \Psi_2(x) \cos \frac{E_1 - E_2}{\hbar} t \right]$$

$$\text{iii) } \langle x \rangle = \int_0^a \Psi^*(x, t) x \Psi(x, t) dx$$

$$= \int_0^a \frac{x}{2} \left[\Psi_1^2(x) + \Psi_2^2(x) + 2 \Psi_1(x) \Psi_2(x) \cos \frac{E_1 - E_2}{\hbar} t \right] dx$$

avg of $\langle x \rangle$ in state 1 and 2.

$$= \frac{1}{2} (\langle x \rangle_1 + \langle x \rangle_2) + \left[\int_0^a x \psi_1(x) \psi_2(x) dx \right] \cos \frac{E_1 - E_2}{\hbar} +$$

$$\left[\int_0^a x \psi_1(x) \psi_2(x) dx \right] = \int_0^a x \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a} dx = \int_0^a \frac{x}{a} (\cos \frac{\pi x}{a} - \cos \frac{3\pi x}{a}) dx$$

Use derivation under
integral sign

$$\int x \cos \beta x dx = \int \frac{d}{d\beta} \sin \beta x dx = \frac{d}{d\beta} \int \sin \beta x dx = \frac{d}{d\beta} \left(-\frac{\cos \beta x}{\beta} \right) = \frac{\cos \beta x + \beta x \sin \beta x}{\beta^2}$$

$$\left[\int_0^a x \psi_1(x) \psi_2(x) dx \right] = \frac{1}{a} \left[\frac{\cos \frac{\pi x}{a} + \frac{\pi x}{a} \sin \frac{\pi x}{a}}{\frac{\pi^2}{a^2}} - \frac{\cos \frac{3\pi x}{a} + \frac{3\pi x}{a} \sin \frac{3\pi x}{a}}{\frac{9\pi^2}{a^2}} \right] \bigg|_0^a = -\frac{16a}{9\pi^2}$$

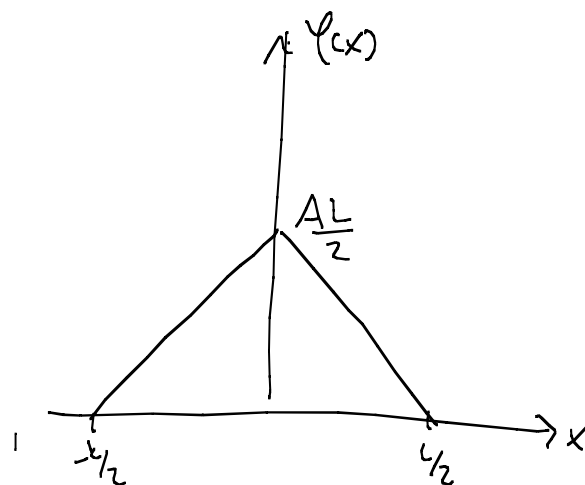
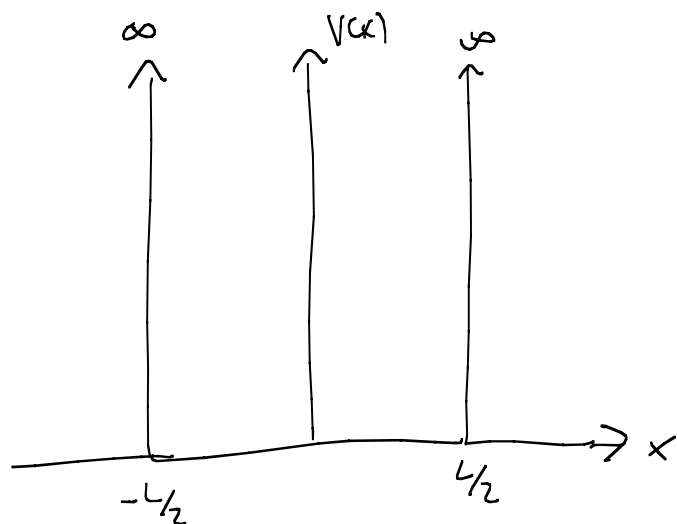
So $\langle x \rangle = \frac{1}{2} (\langle x \rangle_1 + \langle x \rangle_2) - \underbrace{\frac{16a}{9\pi^2}}_{\text{amplitude}} \underbrace{\cos \frac{E_1 - E_2}{\hbar}}_{\text{angular freq.}} +$

$$iv) \Psi(x,t) = A \left(\psi_1(x) e^{-i \frac{E_1}{\hbar} t} + \psi_2(x) e^{-i \left(\frac{E_2}{\hbar} t - \phi \right)} \right), \quad \text{where } A = \frac{1}{\sqrt{2}}$$

$$\begin{aligned} v) |\Psi(x,t)|^2 &= \Psi^*(x,t) \Psi(x,t) \\ &= \frac{1}{2} \left[\psi_1^*(x) \psi_1(x) + \psi_2^* \psi_2 + \psi_1^* \psi_2 e^{i \left[\left(\frac{E_1 - E_2}{\hbar} t - \phi \right) \right]} \psi_2^* \psi_1 e^{-i \left[\left(\frac{E_1 - E_2}{\hbar} t - \phi \right) \right]} \right] \\ &= \frac{1}{2} \left[\psi_1^2(x) + \psi_2^2(x) + 2\psi_1(x) \psi_2(x) \cos \left(\frac{E_1 - E_2}{\hbar} t - \phi \right) \right] \end{aligned}$$

vi) Likewise, oscillations in $\langle x \rangle$ will be phase-shifted by ϕ .

3)



$$a) [\psi] = \frac{1}{\sqrt{\text{distance}}} \quad \left(\int_{-\infty}^{\infty} \psi^* \psi dx = 1 \right)$$

$$[A] \cdot \text{distance} = \frac{1}{\sqrt{\text{distance}}} \Rightarrow [A] = \text{distance}^{-3/2}$$

$$b) \int_{-L/2}^{L/2} \psi^* \psi dx = 2 \int_0^{L/2} A^2 \left(\frac{L}{2} - x \right)^2 dx = 2A^2 \int_0^{L/2} \left(\frac{L^2}{4} - Lx + x^2 \right) dx$$

$$= 2A^2 \left(\frac{L^2 x}{4} - L \frac{x^2}{2} + \frac{x^3}{3} \right) \Big|_0^{L/2}$$

$$= 2A^2 \left(\cancel{\frac{L^3}{8}} - \cancel{\frac{L^3}{8}} + \frac{L^3}{3 \cdot 8} \right) = \frac{A^2 L^3}{12} = 1$$

$$A = \sqrt{\frac{12}{L^3}} = \frac{2\sqrt{3}}{L^{3/2}}$$

$$\textcircled{c} a_n = 2 \int_0^{L/2} A \left(\frac{L-x}{2} \right) \sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L} dx \quad n=1, 3, \dots$$

Wolfram Alpha says:

$$A \int_0^{L/2} 2 \left(\frac{L}{2} - x \right) \cos \left(\frac{n\pi x}{L} \right) dx = \frac{4L^2 \sin^2 \left(\frac{\pi n}{4} \right)}{\pi^2 n^2} A = A \sqrt{\frac{2}{L}} \frac{4L^2 \cdot \frac{1}{2}}{\pi^2 n^2} = \frac{2\sqrt{3}}{L^{3/2}} \frac{\sqrt{2} 2 L^{3/2}}{\pi^2 n^2} = \frac{4\sqrt{6}}{\pi^2 n^2}$$

$$\textcircled{d} E_3 = \frac{\hbar^2 \pi^2 3^2}{2ma^2} = \frac{(6.6 \times 10^{-16} \text{ eV}\cdot\text{s})^2 \pi^2 3^2}{2 \cdot 5.1 \times 10^5 \text{ eV} / (3 \times 10^8 \text{ cm/s})^2 (10^{-7} \text{ cm})^2} = 3.38 \text{ eV}$$

$$\text{probability} = |a_3|^2 = \left(\frac{8\sqrt{6}}{\pi^2 3^2} \right)^2$$