Problem Set 2 – Solutions

1. A. $\psi_1(x) = \dfrac{a^2}{b^2(x-x_0)^2 + c^2}$

$$\int_{-\infty}^{\infty} |\psi_1(x)|^2 dx = a^4 \int_{-\infty}^{\infty} \frac{dx}{\left(b^2(x-x_0)^2 + c^2\right)^2} \qquad \text{let } u = b(x-x_0)$$

$$= \frac{a^4}{b} \int_{-\infty}^{\infty} \frac{du}{\left(u^2 + c^2\right)^2}$$

$$= \frac{a^4}{2bc^2}\left(\left.\frac{u}{c^2+u^2}\right|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{du}{c^2+u^2} \right)$$

$$= \frac{a^4}{2bc^2}\left(\left.\frac{u}{c^2+u^2}\right|_{-\infty}^{\infty} + \frac{1}{c}\arctan \left.\frac{u}{c}\right|_{-\infty}^{\infty} \right)$$

$$= \frac{\pi a^4}{2bc^3}$$

In order to have $\int_{-\infty}^{\infty} |\psi_1(x)|^2 dx = 1$ a must be equal to $\pm \sqrt[4]{\dfrac{2bc^3}{\pi}}$ (or $N = \sqrt{\dfrac{2bc^3}{\pi a^4}}$)

B. $\psi_1(x)$ is even in $(x - x_0)$, therefore $\langle x \rangle = x_0$

$$\langle x^2 \rangle = a^4 \int_{-\infty}^{\infty} \frac{x^2 dx}{\left(b^2 x^2 + c^2\right)^2}$$

$$= \frac{a^4}{b^3} \int_{-\infty}^{\infty} \frac{u^2 du}{\left(u^2 + c^2\right)^2}$$

$$= -\frac{a^4}{b^3}\left. \left(\frac{u}{2(u^2+c^2)} + \frac{1}{2c}\arctan\frac{u}{a} \right)\right|_{-\infty}^{\infty}$$

$$= \frac{a^4 \pi}{2b^3 c} = \frac{c^2}{b^2}$$

$$\langle x^2 \rangle = x_0^2 + \left(\frac{c}{b}\right)^2$$

$$\Delta x = \left(\langle x^2 \rangle - \langle x \rangle^2 \right)^{1/2} = \left| \frac{c}{b} \right|$$

C. $\psi_1(k) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{\infty} \psi_1(x) e^{-ikx} dx$

$$= \frac{1}{\pi}\sqrt{bc^3} \int_{-\infty}^{\infty} \frac{dx e^{-ikx}}{b^2(x-x_0)^2 + c^2}$$

$$= \frac{1}{\pi}\sqrt{\frac{c^3}{b^3}}\int_{-\infty}^{\infty}\frac{dxe^{-ikx}}{(x-x_0)+\frac{c^2}{b^2}}$$

$$= \frac{1}{\pi}\sqrt{\frac{c^3}{b^3}}2\pi i\sum residues$$

$$= 2i\sqrt{\frac{c^3}{b^3}}\sum residues$$

$$\left(x-x_0\right)^2 + \frac{c^2}{b^2} = 0$$

$$x = x_0 \pm i\left|\frac{c}{b}\right|$$

$$= 2i\sqrt{\frac{c^3}{b^3}}\frac{e^{-ik(x_0+i\left|\frac{c}{b}\right|)}}{\left(x_0+i\left|\frac{c}{b}\right|-x_0+i\left|\frac{c}{b}\right|\right)}$$

$= \sqrt{\frac{c}{b}}e^{-ikx_0}e^{k\left|\frac{c}{b}\right|}$ for k<0. Similarly $\psi_1(k) = \sqrt{\frac{c}{b}}e^{-ikx_0}e^{-k\left|\frac{c}{b}\right|}$ for k>0.

$\psi_1(k)$ is even, so $\langle k\rangle = 0$.

$$\left\langle k^2\right\rangle = \left|\frac{c}{b}\right|\int_{-\infty}^{0}k^2e^{2k\left|\frac{c}{b}\right|}dk + \left|\frac{c}{b}\right|\int_{0}^{\infty}k^2e^{-2k\left|\frac{c}{b}\right|}dk$$

$= \frac{1}{2}\int_{-\infty}^{0}\left(\frac{b}{c}\right)^2\frac{1}{4}\varsigma^2e^{\varsigma}d\varsigma - \frac{1}{2}\int_{0}^{\infty}\left(\frac{b}{c}\right)^2\frac{1}{4}\varsigma^2e^{\varsigma}d\varsigma$ and after integration by parts:

$$= \frac{1}{4}\left(\frac{b}{c}\right)^2\left[\varsigma^2e^{\varsigma} - 2\varsigma e^{\varsigma} + 2e^{\varsigma}\right]_{-\infty}^{0}$$

$$= \frac{1}{2}\left(\frac{b}{c}\right)^2$$

$$\Delta k = \left(\left\langle k^2\right\rangle - \left\langle k\right\rangle^2\right) = \frac{1}{\sqrt{2}}\left|\frac{b}{c}\right|$$

2. $\psi_2(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-c^2(x-b)^2} e^{i\alpha(x)} e^{-ikx}$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-c^2(x-b)^2} e^{i(\alpha(x)-kx)}$$

$\alpha(x) - kx$ represents the phase. The function stops oscillating when $\frac{d}{dx}(\alpha(x) - kx) = 0$. Let k' be the wavevector that satisfies this condition. Then we have: $\frac{d\alpha(x)}{dx} = k'$. We can expand $\alpha(x)$ around $x = b$: $\alpha(x) = \alpha(b) + \left(\frac{d\alpha}{dx}\right)_{x=b} (x-b)$. Using $\frac{d\alpha(x)}{dx} = k'$ we have $\alpha(x) = \alpha(b) + k'(x-b)$.

$$\psi_2(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-c^2(x-b)^2} e^{i[\alpha(b)+k'(x-b)-kx]}$$

$$= \frac{1}{\sqrt{2c}} e^{i\alpha(b)} e^{-ikb} e^{\frac{(k'-k)^2}{4c^2}} \text{ (Gaussian centered around } k'\text{).}$$

In order to have it centered around k_0, we need to set $k' = k_0$. Therefore $\alpha(x) = \alpha(b) + k_0(x-b)$ or $\alpha(x) = \alpha_0 + k_0 x$ where α_0 is a constant.

3. Let us divide the space into three regions:

$\psi_I = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$

$\psi_{II} = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}$

$\psi_{III} = 0$

Boundary conditions:

$\psi_I(0) = \psi_{III}(0) \Rightarrow A_1 + B_1 = 0.\ A_1 = -B_1$

$\psi_I(a) = \psi_{II}(a)$

$\frac{d\psi_I(a)}{dx} = \frac{d\psi_{II}(a)}{dx}$

It follows:

$A_1 e^{ik_1 a} - A_1 e^{-ik_1 a} = A_2 e^{ik_2 a} + B_2 e^{-ik_2 a}$

$A_1 k_1 e^{ik_1 a} + A_1 k_1 e^{-ik_1 a} = A_2 k_2 e^{ik_2 a} + B_2 k_2 e^{-ik_2 a}$

$2iA_1 \sin k_1 a = A_2 e^{ik_2 a} + B_2 e^{-ik_2 a}$

$2A_1 k_1 \cos k_1 a = A_2 k_2 e^{ik_2 a} + B_2 k_2 e^{-ik_2 a}$

$$i\frac{k_2}{k_1} \tan k_1 a = \frac{\left(A_2/B_2\right) e^{ik_2 a} + e^{-ik_2 a}}{\left(A_2/B_2\right) e^{ik_2 a} - e^{-ik_2 a}}$$

Let us introduce the following substitution: $\frac{k_2}{k_1}\tan k_1 a = \tan\phi$:

$$i\tan\phi = \frac{\left(A_2/B_2\right)e^{ik_2a} + e^{-ik_2a}}{\left(A_2/B_2\right)e^{ik_2a} - e^{-ik_2a}}$$

$$\left(A_2/B_2\right)e^{ik_2a}i\tan\phi - e^{-ik_2a}i\tan\phi = \left(A_2/B_2\right)e^{ik_2a} + e^{-ik_2a}$$

$$\left(A_2/B_2\right)e^{ik_2a}(i\tan\phi - 1) = e^{ik_2a}(1 + i\tan\phi)$$

$$\left(A_2/B_2\right) = \frac{e^{-ik_2a}}{e^{ik_2a}}\frac{(i\tan\phi + 1)}{(i\tan\phi - 1)}$$

$$\left(A_2/B_2\right) = \frac{e^{-ik_2a}}{e^{ik_2a}}\frac{(i\sin\phi + \cos\phi)}{(i\sin\phi - \cos\phi)} = -e^{-ik_2a+2i\phi} = -e^{2i\delta}$$

where $\delta = \arctan(\frac{k_2}{k_1}\tan k_1 a) - k_2 a$.

$\left|1 - e^{2i\delta}\right|^2 = 2(1 - \cos 2\delta) = 4\sin^2\delta = 4\sin^2\left(\arctan\frac{k_2}{k_1}\tan k_1 a - k_2 a\right)$. If the potential is sufficiently deep and broad the first term dominates and the scattering coefficient becomes:

$\left|1 - e^{2i\delta}\right|^2 = 4\sin^2\arctan\frac{k_2}{k_1}\tan k_1 a = \frac{4}{1 + \left(\frac{k_1}{k_2}\right)^2\cot^2 k_1 a}$. It is obvious that this function shows resonances. (simple identity $\sin^2\arctan y = \frac{y^2}{1 + y^2}$ was used above)

4. A. Solutions that have odd symmetry about x = 0 will have a node at x = 0 and are not affected by the δ-function potential. They are equivalent to the solutions for the infinite well potential.

$$\psi_n = \left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{n\pi x}{L}\right) \qquad n = 2, 4, 6\ldots \qquad \text{and } E_n = \frac{n^2\pi^2}{2}$$

B. $\psi_n(x)_I = N\sin\left[k_n(x + \frac{L}{2})\right]$

$$\psi_n(x)_{II} = -N\sin\left[k_n(x - \frac{L}{2})\right]$$

$$\frac{d\psi_I(0)}{dx} = Nk_n\cos\left[k_n\frac{L}{2}\right]$$

$$\frac{d\psi_{II}(0)}{dx} = -Nk_n\cos\left[k_n\frac{L}{2}\right]$$

$$\Delta \frac{d\psi(0)}{dx} = -2Nk_n \cos\left[\frac{k_n L}{2}\right]$$

Also, $\psi_I(0) = \psi_{II}(0)$

$$-2Nk_n \cos\left[\frac{k_n L}{2}\right] = \frac{2ma}{\hbar^2} N \sin\left[\frac{k_n L}{2}\right]$$

$$\tan\left[\frac{k_n L}{2}\right] = -\frac{k_n \hbar^2}{ma} \text{ and let } a = \frac{400\hbar^2}{Lm}$$

$$\tan\left[\frac{k_n L}{2}\right] = -\left[\frac{k_n L}{2}\right] \cdot \frac{1}{200}$$

An example of a way to solve this trancdendental equation is the following MatLab code:

```
clear
l = 1;
expr(1) = 0;
q = 0;
ar(1) = 0.001;
for n = 0.001:0.5:20;
    l = l + 1;
    ar(l) = n;
    expr(l) = tan(n) + 3*n/200;
    signflag = expr(l)*expr(l-1);
    if signflag < 0
        q = q + 1;
        z = fzero(@funk,[ar(l-1) ar(l)]);
        format long
        solut(q) = 2*z';
        energ(q) = 0.5*solut(q)^2;
    end
end
solut
energy
```

where `funk` is the following function:

```
function y = f(x)
y = tan(x) + 3*x/200;
```

Solutions for k_n and E_n (assuming $L = 1$, $\hbar = 1$ and taking every other solution):

$k_1 = 6.25193$ $E_1 = 19.543$

$k_3 = 12.50387$ $E_3 = 78.173$

$k_5 = 18.75585$ $E_5 = 175.891$

$k_7 = 25.00786$ $E_7 = 312.697$

$k_9 = 31.25994$ $E_9 = 488.592$

Note that there are no crossings between the energy levels, no matter how high a is chosen to be. Since the δ-function potential does not change the number of nodes, it does not change the order of energies.

C. $R_{21,42} = \frac{19.739 - 19.543}{78.957 - 19.739} = 0.00331$

for $a' = a/3$:

$$R_{21,42} = \frac{19.739 - 19.161}{78.957 - 19.739} = 0.01067$$

for $a'' = a/9$:

$$R_{21,42} = \frac{19.739 - 18.085}{78.957 - 19.739} = 0.02793$$

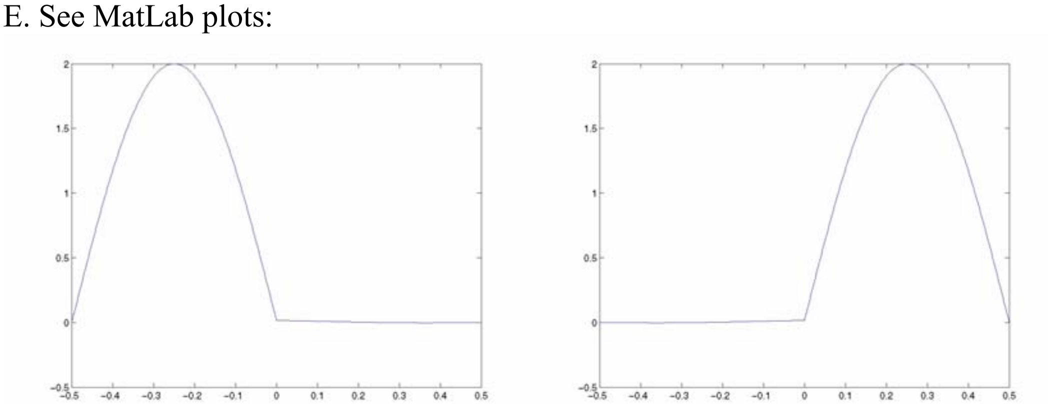
$R_{21,42}$ is proportional to $1/a$.

D. $E_4 - E_3 = 78.957 - 78.173 = 0.784$

$E_2 - E_1 = 19.739 - 19.543 = 0.196$

The spacing is larger as $n \to \infty$. This is the result of the fact that odd-symmetry levels do not change their position while even-symmetry levels shift, where the shift is smaller for larger n. This comes from the probability of finding the particle at x = 0 being smaller for larger n (in absence of the δ-function potential, so these levels are less affected when δ – function potential is present).

E. See MatLab plots:



As can be seen, in order to create a state localized on either side we need to include both even- and odd-symmetry states in the superposition.

F. $\Psi_+(x,t) = 2^{-1/2}\left(\psi_1 e^{-\frac{iE_1 t}{\hbar}} + \psi_2 e^{-\frac{iE_2 t}{\hbar}}\right)$

$$\Psi_+(x,t) = 2^{-1/2}\left(\psi_1 e^{-\frac{iE_1 t}{\hbar}} - \psi_2 e^{-\frac{iE_2 t}{\hbar}}\right)$$

(i) $P_+ = \left|\int dx \Psi_+^*(x,t)\Psi_+(x,0)\right|^2$

$$P_+(t) = \frac{1}{4}\left|\int dx\left(\psi_1 e^{\frac{iE_1t}{\hbar}} + \psi_2 e^{\frac{iE_2t}{\hbar}}\right)(\psi_1 + \psi_2)\right|^2$$

$$= \frac{1}{4}\left|\int dx\left(\psi_1\psi_1^* e^{\frac{iE_1t}{\hbar}} + \psi_2\psi_1^* e^{\frac{iE_2t}{\hbar}} + \psi_1\psi_2^* e^{\frac{iE_1t}{\hbar}} + \psi_2\psi_2^* e^{\frac{iE_2t}{\hbar}}\right)\right|^2$$

$$= \frac{1}{4}\left|e^{\frac{iE_1t}{\hbar}} + e^{\frac{iE_2t}{\hbar}}\right|^2$$

$$= \frac{1}{4}\left|1 + e^{\frac{i(E_1-E_2)t}{\hbar}} + e^{-\frac{i(E_1-E_2)t}{\hbar}} + 1\right|$$

$$= \cos^2\frac{(E_1 - E_2)}{2\hbar}$$

(ii) $P_- = \left|\int dx \Psi_-^*(x,t)\Psi_-(x,0)\right|^2$

$$P_-(t) = \frac{1}{4}\left|\int dx\left(\psi_1 e^{\frac{iE_1t}{\hbar}} - \psi_2 e^{\frac{iE_2t}{\hbar}}\right)(\psi_1 - \psi_2)\right|^2$$

$$= \frac{1}{4}\left|\int dx\left(\psi_1\psi_1^* e^{\frac{iE_1t}{\hbar}} - \psi_2\psi_1^* e^{\frac{iE_2t}{\hbar}} - \psi_1\psi_2^* e^{\frac{iE_1t}{\hbar}} + \psi_2\psi_2^* e^{\frac{iE_2t}{\hbar}}\right)\right|^2$$

$$= \frac{1}{4}\left|1 + e^{\frac{i(E_1-E_2)t}{\hbar}} + e^{-\frac{i(E_1-E_2)t}{\hbar}} + 1\right|$$

$$= \cos^2\frac{(E_1 - E_2)}{2\hbar}$$

(iii) $P_{+-} = \left|\int dx \Psi_+^*(x,t)\Psi_-(x,0)\right|^2$

$$= \frac{1}{4}\left|\int dx\left(\psi_1 e^{\frac{iE_1t}{\hbar}} + \psi_2 e^{\frac{iE_2t}{\hbar}}\right)(\psi_1 - \psi_2)\right|^2$$

$$= \frac{1}{4}\left|\int dx\left(\psi_1\psi_1^* e^{\frac{iE_1t}{\hbar}} - \psi_2\psi_1^* e^{\frac{iE_2t}{\hbar}} + \psi_1\psi_2^* e^{\frac{iE_1t}{\hbar}} - \psi_2\psi_2^* e^{\frac{iE_2t}{\hbar}}\right)\right|^2$$

$$= \frac{1}{4}\left|1 - e^{\frac{i(E_1-E_2)t}{\hbar}} - e^{-\frac{i(E_1-E_2)t}{\hbar}} + 1\right|$$

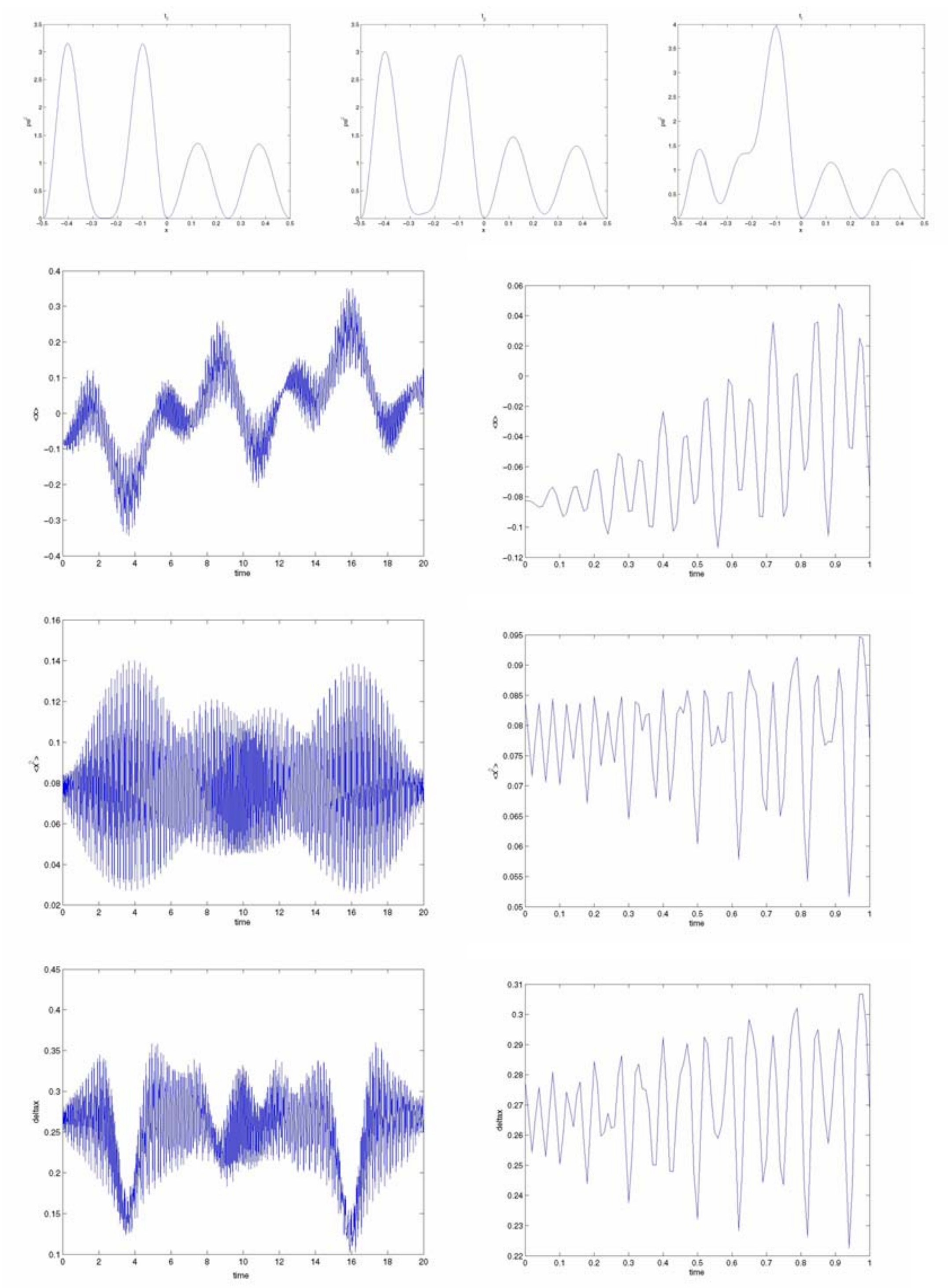
$$= \sin^2\frac{(E_1 - E_2)}{2\hbar}$$

Note that the sum of survival probability of certain state and transfer probability from that state is equal to 1 at all times.

G. The following MatLab code was used to solve this problem:

```
clear
tim = 0;
t1 = 0;
t2 = 1/pi;
t3 = 2*pi/(2*pi^2 - 19.543);
for t = 0:0.001:40;
    tim = tim + 1;
    vreme(tim) = t;
q = 0;
    ek1 = exp(-i*19.543*t);
    ek2 = exp(-i*2*pi^2*t);
    ek3 = exp(-i*78.143*t);
    ek4 = exp(-i*8*pi^2*t);
    ek5 = exp(-i*175.891*t);
    ek6 = exp(-i*18*pi^2*t);
for iks = -0.5:0.001:0;
    q = q + 1;
    psi1(q) = sqrt(2)*sin(6.25193*(iks + 1/2));
    psi2(q) = sqrt(2)*sin(2*pi*iks);
    psi3(q) = sqrt(2)*sin(12.50387*(iks + 1/2));
    psi4(q) = sqrt(2)*sin(4*pi*iks);
    psi5(q) = sqrt(2)*sin(18.75585*(iks + 1/2));
    psi6(q) = sqrt(2)*sin(6*pi*iks);
    psitot(q) = 6^(-1/2)*(psi1(q)*ek1 - psi2(q)*ek2 + psi3(q)*ek3
-
psi4(q)*ek4 + psi5(q)*ek5 - psi6(q)*ek6);
    psisq(q) = psitot(q)*conj(psitot(q));
    coor(q) = iks;
    coord(q) = iks;
end
for iks = 0:0.001:0.5;
    q = q + 1;
    psi1(q) = -sqrt(2)*sin(6.25193*(iks - 1/2));
    psi2(q) = sqrt(2)*sin(2*pi*iks);
    psi3(q) = -sqrt(2)*sin(12.50387*(iks - 1/2));
    psi4(q) = sqrt(2)*sin(4*pi*iks);
    psi5(q) = -sqrt(2)*sin(18.75585*(iks - 1/2));
    psi6(q) = sqrt(2)*sin(6*pi*iks);
    psitot(q) = 6^(-1/2)*(psi1(q)*ek1 - psi2(q)*ek2 + psi3(q)*ek3
-
psi4(q)*ek4 + psi5(q)*ek5 - psi6(q)*ek6);
    psisq(q) = psitot(q)*conj(psitot(q));
    coor(q) = iks;
    coord(q) = iks;
end
coord(q+1) = coord(q) + 0.001;
py(tim) = sum(diff(coord).*psisq);
pyy(tim) = sum(diff(coord).*psisq.*coor);
pyyy(tim) = sum(diff(coord).*psisq.*coor.*coor);
raz(tim) = sqrt(pyyy(tim) - pyy(tim)^2);
end
figure
plot(vreme,raz)
```

```
figure
plot(vreme,pyyy)
figure
plot(vreme,pyy)
```



The motion is composed of fifteen frequencies that are proportional to inverse spacing of the energy levels. These frequencies fall into different groups (3+4+4+4). There are partial recurrences after periods that correspond to these frequencies. Full revival happens after the time that corresponds to time divisible by all the periods. In case of infinite well the frequencies are related by ratios of integers while the relation is not that simple for the well with δ-function. Note that for two superpositions, $\Psi = 6^{-1/2}\left(\Psi_1 - \Psi_2 + \Psi_3 - \Psi_4 + \Psi_5 - \Psi_6\right)$ and $\Psi = 6^{-1/2}\left(\Psi_1 + \Psi_2 + \Psi_3 + \Psi_4 + \Psi_5 + \Psi_6\right)$, $\left\langle x^2 \right\rangle$ and Δx have the same evolution, while $\langle x \rangle$ has opposite sign. The wavepacket defocuses and refocuses while moving between the two parts of the well (tunneling). Crashes of the variance in x correspond to localizations of the wavepacket (times when the six components evolving independently have the highest probability at the same position in space).