SOLUTIONS

PROBLEM SET 3 Due Friday October 14

Physics 115B– FALL 2011

Anecdote:

Hendrik Kramers was once of the important names in quantum mechanics. His work included perturbation theory calculations of the fine structure of the Hydrogen atom, a problem we shall consider in the next week or two. Van Kampen tells a story in "Remembering Kramers":

When Kramers wrote his paper on Brownian motion in 1940 I did not yet know him. Only in 1945, after the war, was it possible for me to go to his lectures without risk of life and limb. Unfortunately, I was not very assiduous, because the newly discovered freedom gave birth to an exuberant student's life. Once I had a celebration that lasted all night and after I came home in the morning I dreamt that I was at a lecture, listening to Kramers. Unfortunately when I woke up it turned out to be true.

Pt assigned Analytic:

10 [1.] Griffiths Problem 4.5

10 [2.] Griffiths Problem 4.8

10 [3.] Write down the Schroedinger equation in a two dimensional circular well: $V(r) = 0$ for $r < a$ and $V(r) = \infty$ for $r > a$. Begin the process of solving it by separation of variables. What can you say about the angular part of the wave function? What equation does the radial part satisfy?

Numeric:

Comment: For the first part of the course, as you develop skill in programming, the computational problems will not necessarily have anything to do with quantum mechanics.

10 [4.] Modify your C or C++ program for the classical harmonic oscillator $F = -kx$ to include an anharmonic term $F = -cx^3$. Can this problem be solved analytically? For the case $c = 0$ you know the period T is independent of the amplitude. Is the same true for $c \neq 0$? Run your program to find out. That is, pick a value of c (it might require a bit of experimentation to find one which most simply illustrates the physics) and then run your code with $v_0 = 0$ and increasingly large values for x_0. Determine T for different x_0. Provide one check on your code by verifying that the maximum velocity the mass attains agrees with energy considerations.

10 [5.] Modify your C or C++ program for the classical harmonic oscillator $F = -kx$ to include a damping term $F = -bv$. Make a plot of $x(t)$ for b nonzero. Can this problem be solved analytically? Can you show your program agrees with the analytic solution?

#1 Griffiths Problem 4.5

Construct $Y_\ell^\ell(\theta,\phi)$ and $Y_3^2(\theta,\phi)$

$$Y_\ell^\ell = (-1)^\ell \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-\ell)!}{(\ell+\ell)!}}\, e^{i\ell\phi} P_\ell^\ell(\cos\theta) = (-1)^\ell \sqrt{\frac{2\ell+1}{4\pi(2\ell)!}}\, e^{i\ell\phi} P_\ell^\ell(\cos\theta)$$

$$P_\ell^\ell(x) = (1-x^2)^{\ell/2}\left(\frac{d}{dx}\right)^\ell \left[\frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell\right]$$

$$= (1-x^2)^{\ell/2}\left[\frac{1}{2^\ell \ell!}\right]\left(\frac{d}{dx}\right)^{2\ell}(x^{2\ell} + b\,x^{2\ell-1} + \dots + 1)$$

$$= (1-x^2)^{\ell/2}\left[\frac{1}{2^\ell \ell!}\right](2\ell)!$$

all terms disappear on differentiation except

$$P_\ell^\ell(\cos\theta) = (1-\cos^2\theta)^{\ell/2}\left[\frac{(2\ell)!}{2^\ell \ell!}\right] = (\sin\theta)^\ell\left[\frac{(2\ell)!}{2^\ell \ell!}\right]$$

$$Y_\ell^\ell = \left[\frac{(-1)(\sin\theta)\,e^{i\phi}}{2}\right]^\ell \left(\frac{1}{\ell!}\right)\sqrt{\frac{(2\ell+1)}{4\pi\,(2\ell)!}}\,(2\ell)!$$

$$\boxed{Y_\ell^\ell = \frac{1}{\ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}\left(-\frac{1}{2}\sin\theta\, e^{i\phi}\right)^\ell}$$

$$Y_3^2 = (-1)^2\sqrt{\frac{7}{4\pi}\frac{1!}{5!}}\, e^{i2\phi}\underbrace{\left[15\sin^2\theta\cos\theta\right]}_{P_3^2(\cos\theta)}$$

$$Y_3^2 = \sqrt{\frac{7}{4\pi\, 5!}}\, 15\sin^2\theta\cos\theta = \frac{1}{4}\sqrt{\frac{7\cdot 3^2\cdot 5^2}{\pi\, 5\cdot 3\cdot 2}}\, e^{i2\phi}\sin^2\theta\cos\theta$$

$$\boxed{Y_3^2 = \frac{1}{4}\sqrt{\frac{105}{2\pi}}\, e^{i2\phi}\sin^2\theta\cos\theta}$$

Show that Y_ℓ^ℓ & Y_3^2 satisfy angular equation:

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)\sin^2\theta\, Y$$

(1) (2) (3)

Let α = coeff of $Y_\ell^\ell = \frac{1}{\ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}} \Rightarrow Y_\ell^\ell = \alpha\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^\ell$

$$\frac{\partial^2 Y_\ell^\ell}{\partial\phi^2} = \frac{\partial}{\partial\phi}\left[\alpha\ell\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^{\ell-1} i\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)\right] = \frac{\partial}{\partial\phi}\left[i\ell\, Y_\ell^\ell\right]$$

$$\Rightarrow \boxed{\frac{\partial^2 Y_\ell^\ell}{\partial\phi^2} = -\ell^2 Y_\ell^\ell} \quad (2)$$

$$\sin\theta\frac{\partial Y_\ell^\ell}{\partial\theta} = \alpha\ell\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^{\ell-1}\left(-\frac{1}{2}\cos\theta e^{i\phi}\right)\sin\theta$$

$$= \ell\left[\alpha\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^\ell\right]\cos\theta = \ell\cos\theta\, Y_\ell^\ell$$

(1)

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y_\ell^\ell}{\partial\theta}\right) = \sin\theta\frac{\partial}{\partial\theta}\left(\ell\cos\theta\,\alpha\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^\ell\right)$$

$$= \sin\theta\left[-\ell\sin\theta\,\alpha\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^\ell + \ell^2\cos\theta\,\alpha\left(-\frac{1}{2}\sin\theta e^{i\phi}\right)^{\ell-1}\left(-\frac{1}{2}\cos\theta e^{i\phi}\right)\right]$$

$$= -\ell\sin^2\theta\, Y_\ell^\ell + \ell^2\cos^2\theta\, Y_\ell^\ell$$

(1) (2)

$$\boxed{-\ell\sin^2\theta\, Y_\ell^\ell + \ell^2\cos^2\theta\, Y_\ell^\ell} + \boxed{-\ell^2 Y_\ell^\ell} = -\ell^2(1-\cos^2\theta)Y_\ell^\ell - \ell\sin^2\theta\, Y_\ell^\ell$$

$$= (-\ell^2-\ell)\sin^2\theta\, Y_\ell^\ell = \underline{-\ell(\ell+1)\sin^2\theta\, Y_\ell^\ell} \quad \boxed{\text{OK}}$$

(3)

So Y_ℓ^ℓ satisfies angular equation. Now for Y_3^2

Again, let α = Coeff. of $Y_3^2 = \frac{1}{4}\sqrt{\frac{105}{2\pi}}$, so $\underline{Y_3^2 = \alpha e^{i2\phi}\sin^2\theta\cos\theta}$

(1)

$$\frac{\partial^2 Y_3^2}{\partial\phi^2} = \frac{\partial}{\partial\phi}\left[2i\alpha\, e^{i2\phi}\sin^2\theta\cos\theta\right] = \boxed{-4\,Y_3^2}$$

$$\sin\theta\,\frac{\partial Y_3^2}{\partial\theta} = \sin\theta\left[\alpha e^{i2\phi}\left(2\sin\theta\cos^2\theta - \sin^3\theta\right)\right]$$

$$= \alpha e^{i2\phi}\left[2\sin^2\theta\cos^2\theta - \sin^4\theta\right]$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial Y_3^2}{\partial\theta}\right) = \sin\theta\,\alpha e^{i2\phi}\left[4\sin\theta\cos^3\theta - 4\sin^3\theta\cos\theta - 4\sin^3\theta\cos\theta\right]$$

$$= 4\alpha e^{i2\phi}\left[\sin^2\theta\cos^3\theta - 2\sin^4\theta\cos\theta\right]$$

$$= 4\left(\alpha e^{i2\alpha}\sin^2\theta\cos\theta\right)\left(\cos^2\theta - 2\sin^2\theta\right)$$

$$= 4\,Y_3^2\left(\cos^2\theta - 2\sin^2\theta\right)$$

$$= \boxed{4Y_3^2\left(1 - 3\sin^2\theta\right)} \quad (2)$$

$$(1) + (2) = -4Y_3^2 + 4Y_3^2\left(1 - 3\sin^2\theta\right)$$

$$= -12\sin^2\theta\, Y_3^2 = -(3)(4)\sin^2\theta\, Y_3^2$$

$$-\left[l\,(l+1)\right] \quad \text{where } \underline{l = 3}$$

So, Y_3^2 satisfies <u>angular equation</u>

#2 Griffiths Problem 4.8

$$A r\, j_1(kr) = \left[\frac{\sin(kr)}{(kr)^2} - \frac{\cos kr}{kr}\right] A r \quad = u(r)$$

Let $V(r)=0$, $l=1$: Radial equation

$$\boxed{\frac{d^2 u(r)}{dr^2} = \left[\frac{2}{r^2} - k^2\right] u(r)} \quad (1)$$

$$u(r) = \frac{A}{k}\left[\frac{\sin(kr)}{kr} - \cos(kr)\right]$$

$$\frac{du}{dr} = \frac{A}{k}\left[\frac{\cos kr}{r} - \frac{\sin kr}{kr^2} + k\sin kr\right]$$

$$\frac{d^2u}{dr^2} = \frac{A}{k}\left[-\frac{k\sin kr}{r} - \frac{\cos kr}{r^2} - \frac{\cos kr}{r^2} + \frac{2\sin(kr)}{kr^3} + k^2\cos(kr)\right]$$

$$= \frac{A}{k}\left[\left(k^2 - \frac{2}{r^2}\right)\cos kr - \left(\frac{k}{r} - \frac{2}{kr^3}\right)\sin(kr)\right] \times \frac{k^2}{k^2}$$

$$\text{LHS of (1)} = Ak\left[\left(1 - \frac{2}{(kr)^2}\right)\cos kr - \left(\frac{1}{kr} - \frac{2}{(kr)^3}\right)\sin(kr)\right]$$

$$= Ak\left[\cos kr - \frac{2\cos kr}{(kr)^2} - \frac{\sin kr}{kr} + \frac{2\sin(kr)}{(kr)^3}\right]$$

$$\text{RHS of (1)} = \left[\frac{2}{r^2} - k^2\right] Ar\left[\frac{\sin(kr)}{(kr)^2} - \frac{\cos kr}{kr}\right]$$

$$= Ak\left[\frac{2}{r} - k^2 r\right]\left[\frac{\sin(kr)}{k^3 r^2} - \frac{\cos kr}{k^2 r}\right]$$

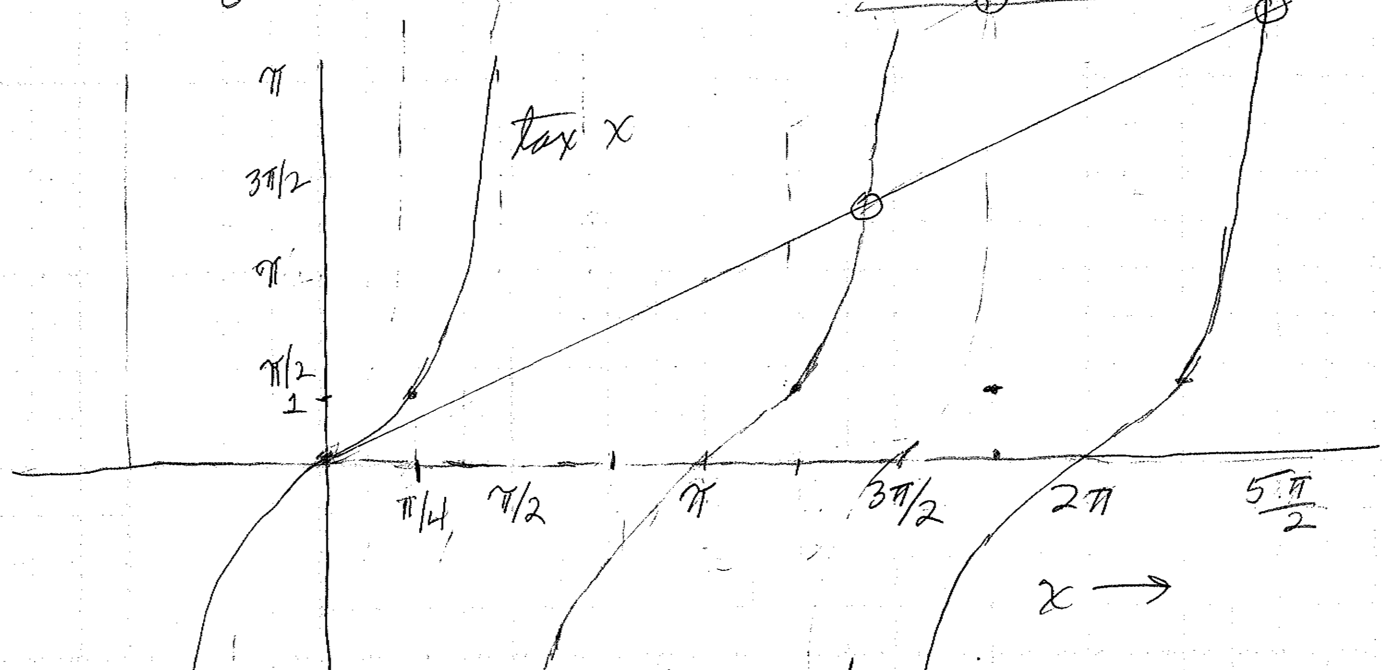
$$= Ak\left[\frac{2\sin(kr)}{(kr)^3} - \frac{\sin(kr)}{(kr)} - \frac{2\cos(kr)}{(kr)^2} + \cos kr\right]$$

So RHS of (1) = LHS of (1) ✓

(#2) Continued 4.8 b

(b) $j_1(x) = 0 \Rightarrow \frac{\sin x}{x^2} - \frac{\cos x}{x} = 0$

or $\sin x = x\cos x \Rightarrow \boxed{x = \frac{\sin x}{\cos x} = \tan x}$



Hard to see roots from graph, so here is numerical solution!

→ Solve using root finder program

Roots for equation: $\boxed{x = \tan x}$

$ka = x \quad k = \frac{x}{a}$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 x^2}{2ma^2}$$

Range	Bessel root #	Value (x)
$\pi \rightarrow 3\pi/2$	1	1.430π
$2\pi \rightarrow 5\pi/2$	2	2.459π
$3\pi \rightarrow 7\pi/2$	3	3.471π
$4\pi \rightarrow 9\pi/2$	4	4.477π
$5\pi \rightarrow 11\pi/2$	5	5.482π
$6\pi \rightarrow 13\pi/2$	6	6.484π
$12\pi \rightarrow 12.5\pi$	12	12.492π

$\Rightarrow x = (n+\frac{1}{2})\pi$

$\Downarrow$

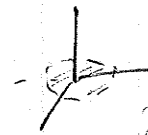
$$\boxed{E = \frac{\hbar^2 (n+\frac{1}{2})^2 \pi^2}{2ma^2}}$$

(#3) Sch Eqn in 2D circular well:

$$V(r) = \begin{cases} 0 & r<a \\ \infty & r>a \end{cases}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi$$

$$\Rightarrow \nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}$$ in <u>polar co-ordinates</u>



$$\Rightarrow \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right]\psi = E\psi}$$

Let $\psi = R(r)\,\Phi(\phi)$ and divide through by ψ

$$\frac{1}{R}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}\right) + \frac{1}{\Phi}\frac{1}{r^2}\frac{\partial^2\Phi}{\partial\phi^2} = -\frac{2mE}{\hbar^2}$$

Mult by r^2

depends only on r depends only of ϕ

$$\underbrace{\left[\frac{r}{R}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}\right) + \frac{2mE}{\hbar^2}r^2\right]}_{=m^2} + \underbrace{\left[\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2}\right]}_{=-m^2} = 0$$

Angular Part: $$\boxed{\frac{\partial^2\Phi}{\partial^2\phi^2} = -m^2\Phi \Rightarrow \Phi(\phi) = e^{im\phi} \quad m = 0, \pm 1, \pm 2.}$$

Radial Equation: $$\boxed{r^2\frac{\partial^2 R}{\partial^2 r} + r\frac{\partial R}{\partial r} + \left(\frac{2mE}{\hbar^2}r^2 - m^2\right)R = 0}$$

No obvious analytical solution to <u>radial equation</u>

(#4) For my model:

$k = 1.0, \; m = 1.0, \; c = 2.0, \; x_0 = (1.5, 3.0, 5.0)$

<u>DE</u>: $m\ddot{x} = -kx - cx^3$

2^{ND} order <u>non-linear</u> DE $\Rightarrow$ No analytical model

<u>Case 1</u>: $c = 0$

$$T = 1/f = \frac{2\pi}{\sqrt{\frac{k}{m}}} = \underline{\underline{2\pi}} \qquad \underline{\underline{A = 1.5}}$$

<u>Case 2</u>: For $c = 2.0$, we vary amplitude:

c	x_0	T	Maximum V	Max Computed V (below)
2.0	1.5	3.0	2.7	2.70
2.0	3.0	1.6	9.6	9.49
2.0	5.0	0.9	26.1	25.5

So, larger x_0 (amplitude) means a <u>shorter</u> period (<u>T is not independent</u> of x_0)

<u>Energy & velocity calculation</u>:

$$F = -kx - cx^3 = -\frac{\partial V}{\partial x} \Rightarrow V = \int kx + cx^3 = \frac{1}{2}kx^2 + \frac{1}{4}cx^4$$

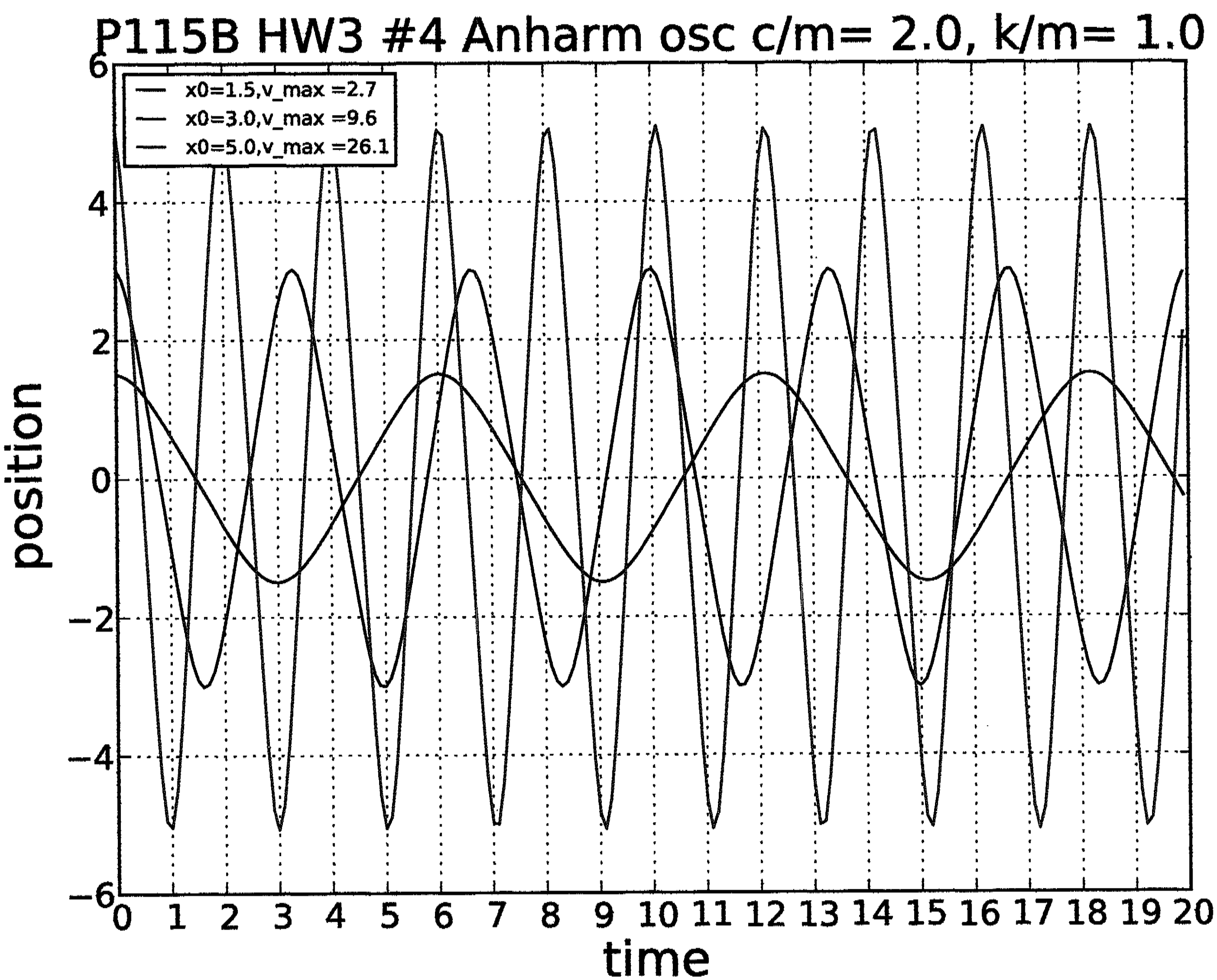
So, for a maximum velocity:

$$\frac{1}{2} m V_{max}^2 = \frac{1}{2} k x_{max}^2 + \frac{1}{4} c x_{max}^4$$

$$V_{max} = \left(\left(\frac{k}{m}\right) x_{max}^2 + \frac{1}{2}\left(\frac{c}{m}\right) x_{max}^4 \right)^{1/2}$$

Max. instantaneous V is close to <u>theoretical</u> max. If time interval were smaller (dt), then actual max velocity values get <u>closer</u> to theoretical values.

#4


P115B HW3 #4 Anharm osc c/m= 2.0, k/m= 1.0
x0=1.5,v_max =2.7
x0=3.0,v_max =9.6
x0=5.0,v_max =26.1
position
time
6
4
2
0
−2
−4
−6
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

8

#5 For my model:

$x_0 = 2.0$, $V_0 = 0$, $k = 1.0$, $m = 1.0$, $b = (0, .25, 1, 2)$

Case 1: $b = 0$ $\quad T = 1/f = \frac{2\pi}{\sqrt{k/m}} = 2\pi \approx 6.2$ ✓

$f = \omega / 2\pi$

DE: $\quad m\ddot{x} = -kx - b\dot{x}$ $\quad \left\{ \begin{array}{l} k = 1 \\ m = 1 \\ b \text{ varies} \end{array} \right\}$

$\ddot{x} + b\dot{x} + 1x = 0$ $\quad \lambda = \frac{-b \pm \sqrt{b^2 - 4}}{2}$

General analytical solution:

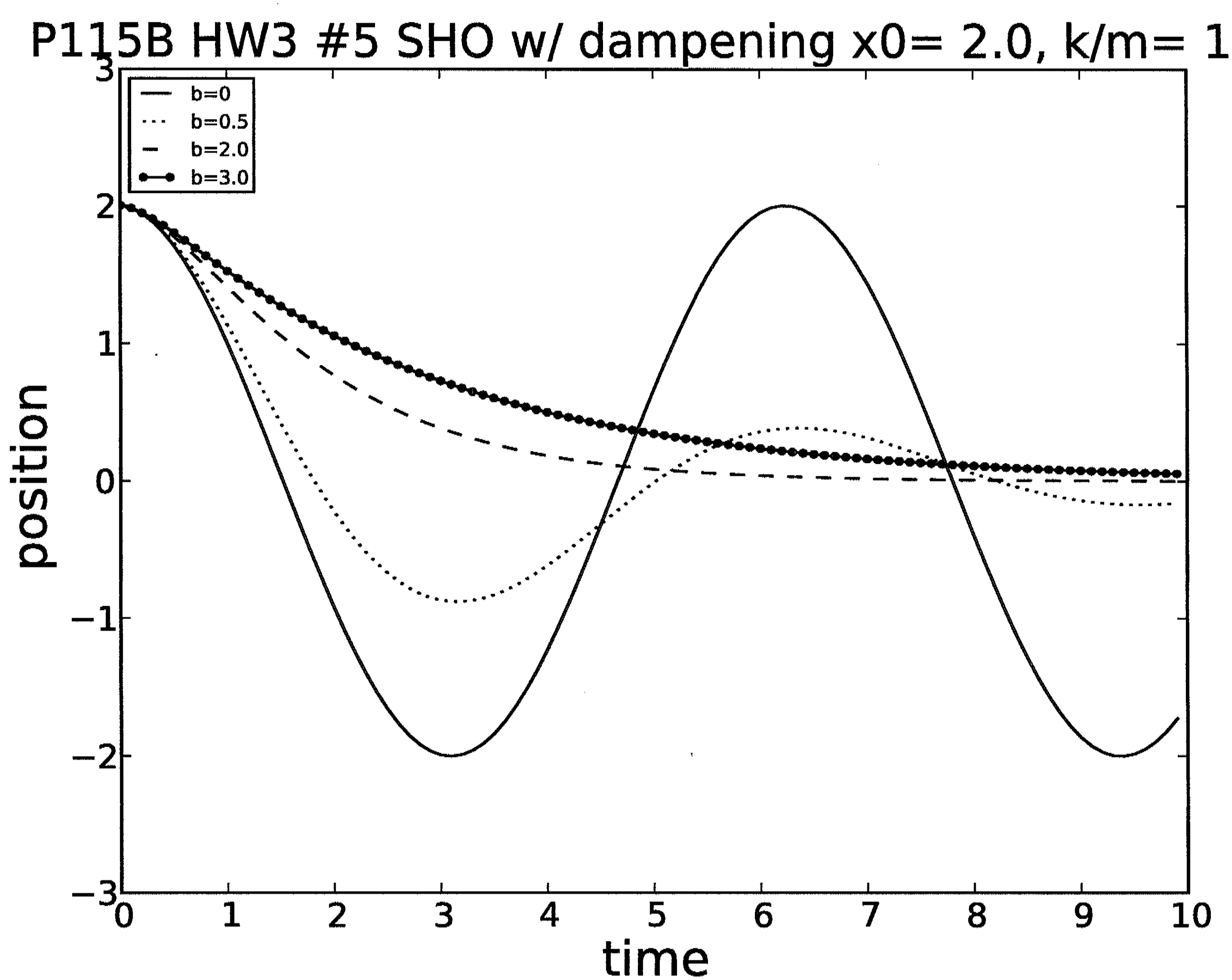
$b < 2 \quad 2e^{-b/2\,t} \cos\left(\left(|b^2-4|\right)^{1/2} t\right)$ underdamped

$b = 2 \quad 2e^{-b/2\,t}$ critical dampening

$b > 2 \quad 2e^{\left(-b/2 \pm \frac{1}{2}\sqrt{b^2-4}\right)t}$ over-damped

b	Type	Behavior
0	No dampening	No decay
.5	Underdamped	Decays after many cycles
2.00	Critical dampening	Decays in 1^{st} or 2^{ND} cycle
3.0	Overdamped	Decays in 1^{st} cycle

Graph agrees with analytical model


P115B HW3 #5 SHO w/ dampening x0= 2.0, k/m= 1.0
b=0
b=0.5
b=2.0
b=3.0
position
time
3
2
1
0
−1
−2
−3
0
1
2
3
4
5
6
7
8
9
10

#5

(10)

```
//
//  P115B  HW3  #4
//
//  Program to implement Molecular Dynamics
//    with Leapfrog method
//  Adds anharmonic term f = -c * x^3
#include <iostream>
#include <fstream>
#include <math.h>
using namespace std;
double c, k,m, xn, xn_m1, vn, vn_m1,x0, v0,  dt ;
int num_periods;
int main()
{
   c = 1.0;
   k  = 3.0;
   m =  1.0;
   x0 = 1.5;
   v0 = 0.0;
   dt = .1;
   num_periods = 100;
// Set up disk file for output
   ofstream fout("HW3-4_out1.dat");
   fout << "  t      x(t)        v(t)"  << endl;
// Generate data with leapfrog
   xn_m1 = x0;
   vn_m1 = v0;
   for ( int i= 0; i< num_periods; i++)
   {
      xn = xn_m1 + vn_m1 * dt;
      vn = vn_m1 - (k/m)*xn * dt - (c/m) * pow(xn,3)* dt;
      fout << "  "<< i + 1 << '\t' << xn << '\t' << vn <<endl;
      xn_m1 = xn;
      vn_m1 = vn;
   }
   cout << " Finished writing data to file" << endl;
   return 0;
}
```

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```
//
//  P115B  HW3  #5
//
//  Program to implement Molecular Dynamics
//    with Leapfrog method
//  Adds dampening term f = -(b/m) * v
#include <iostream>
#include <fstream>
#include <math.h>
using namespace std;
double c, k,m, xn, xn_m1, vn, vn_m1,x0, v0,  dt ;
int num_periods;
int main()
{
   c = 1.0;
   k  = 1.0;
   m =  1.0;
   x0 = 1.5;
   v0 = 0.0;
   dt = .1;
   num_periods = 100;
// Set up disk file for output
   ofstream fout("HW3-5_out1.dat");
   fout << "  t      x(t)        v(t)"  << endl;
// Generate data with leapfrog
   xn_m1 = x0;
   vn_m1 = v0;
   for ( int i= 0; i< num_periods; i++)
   {
      xn = xn_m1 + vn_m1 * dt;
      vn = vn_m1 - (k/m)*xn * dt - (b/m) * vn_m1* dt;
      fout << "  "<< i + 1 << '\t' << xn << '\t' << vn <<endl;
      xn_m1 = xn;
      vn_m1 = vn;
   }
   cout << " Finished writing data to file" << endl;
   return 0;
}
```

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