SOLUTIONS

PROBLEM SET 4 Due Friday October 21

Physics 115B– FALL 2011

Analytic:

10 [1.] Griffiths Problem 4.13

10 [2.] Griffiths Problem 4.14

10 [3.] Griffiths Problem 4.16

10 [4.] The diffusion equation decribes the spreading of particles, heat, etc and is sometimes referred to as the 'imaginary time Schroedinger equation' since the two look very similar with the replacement $t \leftrightarrow it$. In the absence of a source, the diffusion equation is,

$$D\,\nabla^2\Psi(\vec{r},t) = \frac{\partial}{\partial t}\Psi(\vec{r},t)$$

D is the 'diffusion constant'. When D is large, the spreading is rapid. Solve the diffusion equation in one dimension for $\Psi(x,t)$ given $\Psi(x,t=0) = \delta(x)$. Also, give the general solution for any $\Psi(x,t=0)$. Hint: The mathematics is basically identical to the discussion of the free particle Schroedinger equation in Griffiths Sec. 2.4.

10 [5.] Now consider the diffusion equation in 3D, with a source,

$$(D\nabla^2 + \lambda)\Psi(\vec{r},t) = \frac{\partial}{\partial t}\Psi(\vec{r},t)$$

The λ term represents, for example, a uniform source of heat in a material, and $\Psi(\vec{r},t)$ would be the temperature at position $\vec{r}$ and time t. In this problem, we are going to see under what conditions a block of material will melt. The physical picture is that the $D\nabla^2$ term helps prevent melting by diffusing the heat away, whilst the λ term tries to increase the temperature. We need to see which effect wins. Begin to solve this diffusion equation by separating out the time dependence $\Psi(\vec{r},t) = R(\vec{r})g(t)$. How does $g(t)$ differ from the $e^{-iEt/\hbar}$ encountered for the Schroedinger equation? Finish solving the equation for a cubical block of material $0 < x, y, z < a$. What is the melting condition? Hint: You need to keep $g(t)$ from diverging!

10 [6.] Solve the 3D diffusion equation with a source, as in problem 5, but for a sphere of material of radius $r = a$ instead of a cube. This problem is basically identical to the spherical well Schroedinger equation discussed in class. Again, determine the melting condition. Compare with the melting condition of Problem 5. Which is more prone to melt, a sphere of volume V or a cube of volume V? Why? Comment: Problems 5,6 have an important application, namely to the computation of the critical shape and mass of uranium needed for the core of a power plant to melt.

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.

#1 Griffiths Prob. 4.13

(a) Ground state $\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$ $\quad 4\pi$

$$\langle r \rangle = \int \psi_{100}^* \, r \, \psi_{100} = \frac{1}{\pi a^3}\left[\int_0^\infty e^{-2r/a} r^3 \, dr\right]\left[\int_0^{2\pi} d\phi\right]\left[\int_0^\pi \sin\theta \, d\theta\right]$$

$$= \frac{4\pi}{\pi a^3}\left[\frac{3!}{\left(\frac{2}{a}\right)^4}\right] = \frac{4}{a^3}\left(\frac{6a^4}{2^4}\right) = \boxed{\frac{3}{2} a}$$

$$\langle r^2 \rangle = \frac{1}{\pi a^3}\left[\int_0^\infty e^{-2r/a} r^4 \, dr\right] 4\pi = \frac{4}{a^3}\left(\frac{4!}{\left(\frac{2}{a}\right)^5}\right) = \frac{4^2 6 a^2}{2^5} = \boxed{3a^2}$$

(b) Ground state is symmetric about origin for $x, y, \& z$

$\langle x \rangle = 0$ (average value of x component is zero)

$$\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = 3\langle x^2 \rangle$$

$$\langle x^2 \rangle = \frac{1}{3}\langle r^2 \rangle = \boxed{a^2}$$

(c) $x = r \sin\theta \cos\phi$ $\quad R_{21} \quad Y_1^1$

$$\psi_{211} = R_{21} Y_1^1 = \left(\frac{a^{-3/2}}{\sqrt{24}} \frac{r}{a} e^{-r/2a}\right) - \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \, e^{i\phi}$$

$$= -\frac{1}{\sqrt{64 \pi a^5}}[\;] = -\frac{1}{8a^2}\frac{1}{\sqrt{\pi a}} \, r \, e^{-r/2a} \sin\theta \cos\phi$$

$$\langle x^2 \rangle = \frac{1}{\pi a}\frac{1}{(64a^5)}\left[\int (r^2 e^{-r/a} \sin^2\theta) (r^2 \sin^2\theta \cos^2\phi)(r^2 \sin\theta) \, dr \, d\theta \, d\phi\right]$$

$$= \frac{1}{\pi 64 a^5}\left[\int_0^\infty r^6 e^{-r/a} dr\right]\left[\int_0^\pi \sin^5\theta \, d\theta\right]\left[\int_0^{2\pi} \cos^4\phi \, d\phi\right]$$

$$= \frac{1}{64\pi a^5}\left[\frac{6!}{\left(\frac{1}{a}\right)^7}\right]\left[\frac{16}{15}\right]\left[\star\right] = \frac{a^2 \, 6\cdot5\cdot3\cdot2}{3\cdot5} = \boxed{12a^2}$$

4 $\quad$ 4.4 $\quad$ 3.5

#2 <u>Griffiths 4.14</u>

For ψ_{100} find most probable value of r

$$P(r) = 4\pi |\psi_{100}|^2 r^2 = \frac{4\pi}{\pi a^3} e^{-2r/a} r^2$$

Most probable when $\frac{\partial P}{\partial r} = 0$

$$\frac{\partial P}{\partial r} = \frac{4}{a^3}\left[-\frac{2}{a} e^{-2r/a} r^2 + 2r e^{-2r/a}\right] = 0$$

$$\Rightarrow 2r e^{-2r/a}\left[-\frac{r}{a} + 1\right] = 0$$

$\Rightarrow$ $\boxed{r = a}$ is most probable r

(#3) Griffiths Prob # 4.16

For hydrogenic atom,

$$E_n(Z) = \frac{m}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2\frac{1}{n^2} = Z^2\frac{m}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{n^2} = \underline{\underline{Z^2E_n}}$$

$$E_1(Z) = \boxed{Z^2E_1}$$

$$a(Z) = \frac{4\pi\varepsilon_0\hbar^2}{m(Ze)e} = \boxed{a/Z}$$

$$R(Z) = \frac{m}{4\pi c\hbar^3}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2 = \boxed{Z^2R}$$

For Lyman series $\quad \frac{1}{\lambda_n} = R\left(1 - \frac{1}{n^2}\right)$

$$\frac{1}{\lambda_2} = \frac{3}{4}R \Rightarrow \lambda_2 = \frac{4}{3}\left(\frac{1}{R}\right) \qquad \lambda_1 = \frac{1}{R}$$

$R(Z) = Z^2R$ (above), so for Lyman series

$$Z=2 \quad \lambda_1 \approx \frac{1}{4R} = \frac{1}{4(1.1\times10^7)} \approx 2.3\times10^{-8}\,m \quad \boxed{UV}$$

$$Z=3 \quad \lambda_1 = \frac{1}{9R} \quad \frac{1}{9(1.1\times10^7)} \approx 10^{-8}\,m \quad \boxed{UV}$$

#4 $\quad D\,\dfrac{\partial^2\psi}{\partial x^2}(x,t) = \dfrac{\partial}{\partial t}\psi(x,t)$

Let $\psi(x,t) = f_1(x)g(t) \Rightarrow \dfrac{D}{f}\dfrac{d^2f}{dx^2} = \dfrac{1}{g}\dfrac{dg}{dt} = -k^2$ (constant)

so $g(t) = e^{-k^2 t}$

$$\frac{d^2 f}{dx^2} = -\frac{k^2}{D} f \Rightarrow f(x) = A e^{-i\left(\frac{k}{\sqrt{D}}\right)x}$$

$$\psi(x,t) = fg = A e^{-i\frac{k}{\sqrt{D}}x - k^2 t} \quad \text{(Plane wave)}$$

FT $\quad \boxed{\psi(x,t) = \dfrac{1}{\sqrt{2\pi}}\displaystyle\int_{-\infty}^{\infty}\phi(k)\, e^{-i\frac{kx}{\sqrt{D}} - k^2 t}\, dk}$ $\quad$ $\boxed{\text{General solution}}$

$$\psi(x,0) = \delta(x)$$

$$\Rightarrow \phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\underbrace{\psi(x,0)}_{\delta(x)}\, e^{-i\frac{k x}{\sqrt{D}}}\,dx = \frac{1}{\sqrt{2\pi}}$$

$$\boxed{\psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\frac{ik}{\sqrt{D}}x - k^2 t}\, dk}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\left[k\sqrt{t} + \frac{ix}{2\sqrt{Dt}}\right]^2 - \left(\frac{x^2}{4Dt}\right)} dk \qquad \boxed{\text{Completing square}}$$

Let $u = k\sqrt{t} + \dfrac{ix}{2\sqrt{Dt}} \Rightarrow du = \sqrt{t}\, dk$

$$\psi(x,t) = \frac{1}{2\pi} e^{-x^2/4Dt}\underbrace{\int_{-\infty}^{\infty} e^{-u^2}}_{=\sqrt{\pi}}\frac{du}{\sqrt{t}} = \boxed{\frac{1}{2\sqrt{\pi t}}\, e^{-x^2/4Dt}} \quad \text{Unique Solution}$$

$\psi(x,t)$ is a Gaussian wave that spreads spatially with time

#5 $\quad (D\nabla^2 + \lambda)\,\Psi(\vec{r},t) = \frac{\partial}{\partial t}\Psi(\vec{r},t)$

Let $\Psi(\vec{r},t) = R(\vec{r})\,g(t) \Rightarrow \underbrace{\frac{1}{R}(D\nabla^2+\lambda)R}_{①} = \underbrace{\frac{1}{g(t)}\frac{\partial g(t)}{\partial t}}_{②} = -\alpha$ (constant)

② So $\frac{dg(t)}{dt} = -\alpha g(t)$ and $\boxed{g(t) = e^{-\alpha t}}$

$g(t)$ is (normally) a decaying exponential vs oscillating as in Sch. Eqn ($e^{-iEt/\hbar}$)

For ① $\quad (D\nabla^2+\lambda)R = -\alpha R$

$$\Rightarrow \quad \nabla^2 R = -\left(\frac{\lambda+\alpha}{D}\right)R$$

Soln is:

$$R(x,y,z) = A\sin(k_x x)\sin(k_y y)\sin(k_z z) \quad \text{in } 3\,D$$

For cube such that $0 < x, y, z < a$

$$R(x,y,z) = \left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right)$$

$$D\nabla^2 R + (\lambda+\alpha)R = \left[-D\frac{\pi^2}{a^2}(n_x^2+n_y^2+n_z^2) + \lambda + \alpha\right]R = 0$$

or $\alpha = -\lambda + \frac{D\pi^2}{a^2}(n_x^2+n_y^2+n_z^2)$

Melting condition is if $\alpha < 0$, causing $g(t)$ to have exponential growth
This means $\alpha \geq 0$ or $-\lambda + \frac{D\pi^2}{a^2}(n_x^2+n_y^2+n_z^2) > 0$

Critical state is $n_x = n_y = n_z = 1 \Rightarrow \frac{D\pi^2}{a^2}(3) > \lambda$

or $\boxed{a < \left(3\frac{D\pi^2}{\lambda}\right)^{1/2} \text{ for cube not to melt.}}$

Critical Volume of cube $= a^3 = \left(\frac{3D\pi^2}{\lambda}\right)^{3/2}$

#6 Following notes (on-line)

$[D\nabla^2 + \lambda + \alpha]\, u(r) = 0$ for ∇^2 = Spherical Laplacian

Let $u(r) = R(r)\, Y(\theta,\phi)$, equation reduces to angular equation with solution $Y_\ell^m(\theta,\phi)$ and "radial" equation:

$$\frac{1}{R}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{r^2(\lambda+\alpha)}{D} = \ell(\ell+1)$$

$$\Rightarrow \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{r^2}{D}[\lambda+\alpha]R = \ell(\ell+1)R$$

Let $u(r) = r\,R(r)$

$$\Rightarrow \frac{d^2u}{dr^2} + \left[\frac{\lambda+\alpha}{D} - \frac{\ell(\ell+1)}{r^2}\right] u = 0$$

Solutions are spherical Bessel functions ($j_\ell(kr)$) of order ℓ where $k^2 = \frac{\lambda+\alpha}{D}$

At $r \to a$, $j_\ell(kr) \to 0 \Rightarrow ka = \beta_{n\ell}$ (n^{th} root of j_ℓ)

$$\Rightarrow \sqrt{\frac{\lambda+\alpha}{D}}\, a = \beta_{n\ell} \quad \text{or} \quad \boxed{\alpha = -\lambda + \frac{D\beta_{n\ell}^2}{a^2} > 0}$$

For $\alpha > 0$, most critical mode is smallest $\beta_{n\ell}$. In this case ($\ell = 0$), $\beta_{10} = \pi$.

$$\Rightarrow \frac{D\pi^2}{a^2} > \lambda \Rightarrow a \leq \left(\frac{D\pi^2}{\lambda}\right)^{1/2}$$

For sphere, $V_{crit} = \frac{4}{3}\pi a^3 = \frac{4}{3}\pi\left(\frac{D\pi^2}{\lambda}\right)^{3/2}$

For cube, $V_{crit} = a^3 = \left(3\frac{D\pi^2}{\lambda}\right)^{3/2} = 3^{3/2}\left(\frac{D\pi^2}{\lambda}\right)^{3/2}$

$V_{crit}^{sph} < V_{crit}^{cube}$ Sphere is more prone to melt, since sphere is "tightest" way to arrange 3D material

6

[7.] Write a C or C++ program to solve the Kepler problem by molecular dynamics. You need to keep track of position and velocity in two dimensions. The heart of your code is

20

$$
\begin{aligned}
x &= x + v_x\, dt \\
y &= y + v_y\, dt \\
r &= \sqrt{x^2 + y^2} \\
v_x &= v_x - \frac{GM_{\text{sun}}\, x}{r^3}\, dt \\
v_y &= v_y - \frac{GM_{\text{sun}}\, y}{r^3}\, dt
\end{aligned}
$$

Explain where the equations for v_x and v_y come from. Why is there an r^3 in the denominator?! Generate a few orbits (e.g. circular, parabolic) to test your code.

$$F = -\frac{G M_{sun} m_{sat}}{r^2}\hat{r} = m_{sat}\,\bar{a}_{sat}$$

$$\text{So} \quad \bar{a}_{sat} = -\frac{GM_{sun}}{r^2}\left(\frac{\bar{r}}{r}\right) \qquad \bar{r} = x\hat{x} + y\hat{y}$$

$$a_x = -\frac{GM_{sum}}{r^3}x \qquad V_x = V_x - \frac{GM_{SUN}}{r^3}x\,dt$$

$$a_y = -\frac{GM_{SUN}}{r^3}y \qquad V_y = V_y - \frac{GM_{SUN}}{r^3}y\,dt$$

#7 Numeric:

Attached are C program and polar co-ordinate plots of several orbitals.

Program uses astronomical units (AU) for convenience:

1 AU distance = 1 earth-Sun distance $\sim 1.5 \times 10^{11}$ m

~~1~~ AU mass = 1 Sun mass $\sim 2.0 \times 10^{20}$ kg

1 AU time = 1 year - time for satellite (earth) to orbit Sun-mass at radius of 1 AU

For circular orbit, we have:

$$m\frac{v^2}{r} = \frac{GMm}{r^2} \Rightarrow v = \sqrt{\frac{GM}{r}}$$

So and $T = \frac{2\pi r}{v} = \frac{2\pi r^{3/2}}{\sqrt{GM}}$

In AU units $T=1$, $r=1$, so

$$1 = \frac{2\pi}{\sqrt{GM}} \Rightarrow \boxed{GM_{sun} = 4\pi^2}$$ which is used in program

Where do v_x & v_y & r^3 come from?

$$F = -\frac{GM_{SUN}m_{sat}}{r^2}\hat{r}_{\text{(unit vector)}} = -\frac{GM_{sun}m_{sat}}{r^2}\left(\frac{\bar{r}}{r}\right) = -\frac{GM_{SUN}m_{sat}}{r^3}\overbrace{(x\hat{x} + y\hat{y})}^{\bar{r}}$$

$$\bar{a}_x = -\frac{GM_{SUN}}{r^3}x\hat{x} \Rightarrow \boxed{v_x = v_x - \frac{GM_{SUN}}{r^3}x * dt}$$

$$\bar{a}_y = -\frac{GM_{SUN}}{r^3}y\hat{x} \Rightarrow \boxed{v_y = v_y - \frac{GM_{SUN}}{r^3}y * dt}$$

```
//
//  P115B  HW4  7
//   g++ -o kepler.exe kepler.c
//  Program to to solve Kepler problem
//   with Molecular Dynamics
#include <iostream>
#include <fstream>
#include <math.h>
using namespace std;
int main()
{
   double xn_m1, yn_m1, vnx_m1, vny_m1;
//  Assign constants
//
    const int num_steps = 200;
    const double pi = 3.1415926;
    double GM = 4 * pi * pi;   // gravity constant * mass of sun ( in AU^3/yr^2)
    double mass_planet = .001; // in solar masses
    double x0  = 1.0;          // Initial position (in AU)
    double y0  = 0.0;
    double vx0 = 0.0;
    double vy0 = 2.5 * pi;     // Initial velocity (tangential)
    double dt = .005;          // time step in years
// Arrays for variables
//
    double time_array[num_steps];
    double xn[num_steps];          // x position for step
    double yn[num_steps] ;         // y position for step
    double vnx[num_steps] ;        // x velocity for steps
    double vny[num_steps]  ;       // y velocity for steps
    double theta_array[num_steps]; // holds angle for polar co-ordinates
    double r_array[num_steps];     // holds radius for polar co-ordinates
// Generate data with leapfrog
//
    xn_m1 = x0;
    yn_m1 = y0;
    vnx_m1 = vx0;
    vny_m1 = vy0;
    for (int i = 0; i < num_steps; i++)
        {
        double accel,vel_square,r, r_cube;
        xn[i] = xn_m1 + vnx_m1 * dt;
        yn[i] = yn_m1 + vny_m1 * dt;
        r = sqrt( xn[i]*xn[i] + yn[i]*yn[i]);
        r_cube = r * r *r;
        accel = (GM * dt)/r_cube;
        vnx[i] = vnx_m1 - accel * xn[i];
        vny[i] = vny_m1 - accel * yn[i];
        xn_m1 = xn[i];
        yn_m1 = yn[i] ;
        vnx_m1 = vnx[i];
        vny_m1 = vny[i] ;
        time_array[i] = i * dt;
        r_array[i] = r;
        theta_array[i] = atan2( yn[i],xn[i]);
        }
// Set up disk files for output
    ofstream fout("kepler_out1.dat");
    fout << "  t         x        y         vx        vy      r      theta   " << endl;
    for (int i = 0; i <num_steps; i++)
    {
      fout << time_array[i]<< "   " << xn[i]<< "   " << yn[i]<< "   " << vnx[i]<< "   " << vny[i]<< "   " <<
r_array[i]<< "   " << theta_array[i]  <<endl;
     }
cout << " Finished writing data to file" << endl;
   return 0;
}
```

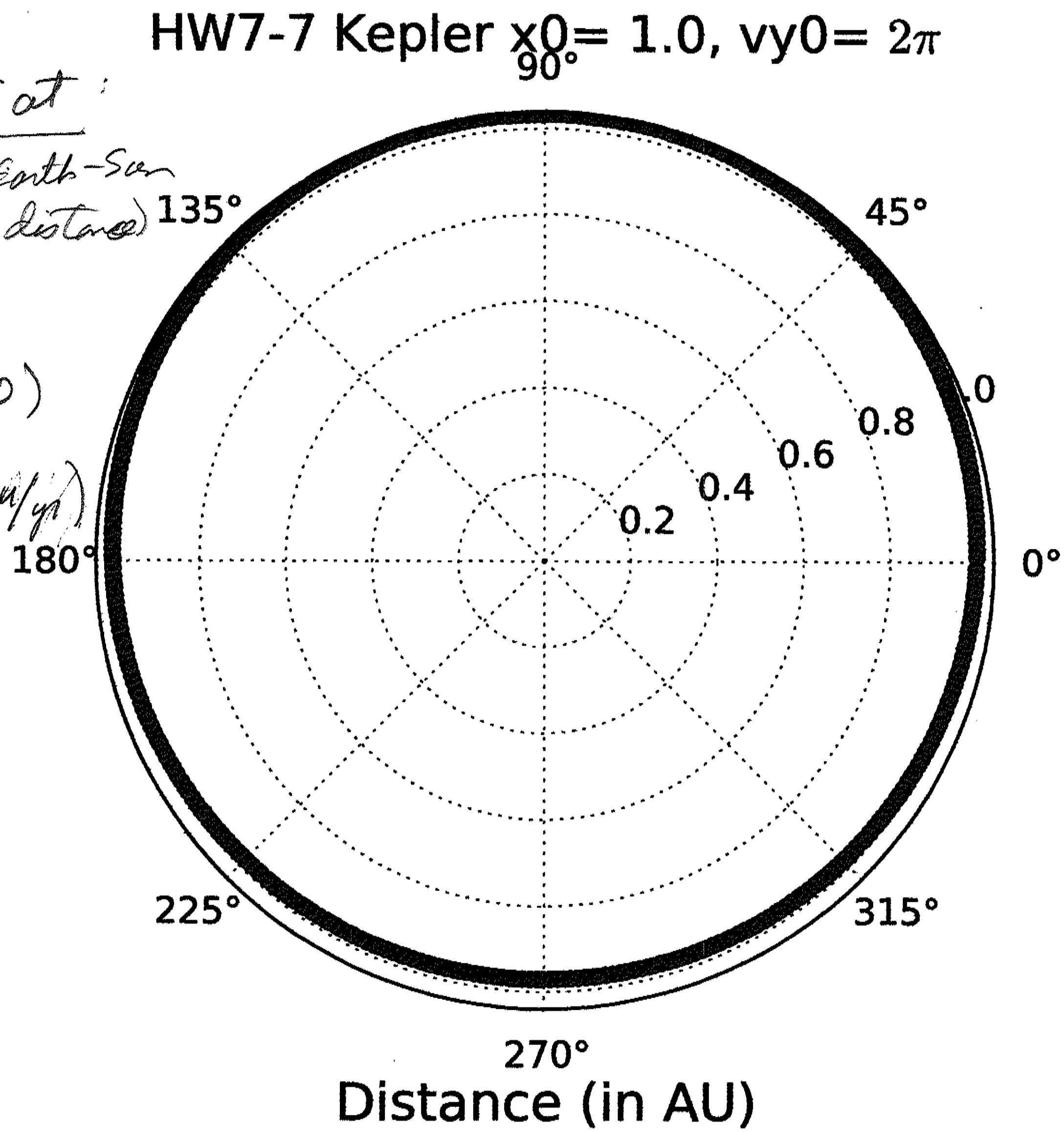
Near circular orbit at:

radius = 1 AU (Earth-Sun distance)

Initial position/velocity

$(x_0, y_0) = (1\,AU, 0)$

$(v_{x0}, v_{y0}) = (0, 2\pi\ AU/yr)$



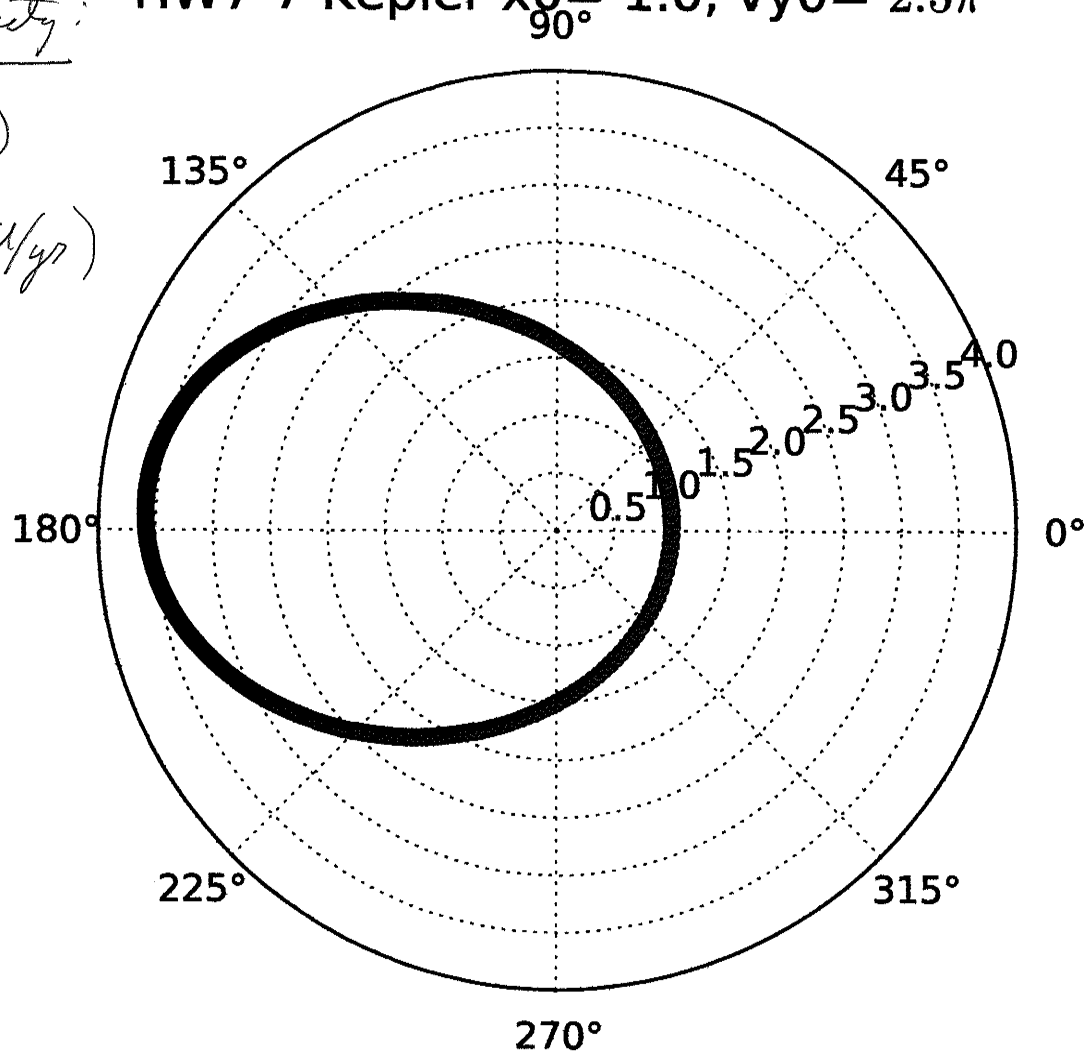
Elliptical Orbit

Initial position/velocity:

$(x_0, y_0) = (1 \text{ AU}, 0)$

$(v_x, v_y) = (0, 2.5\pi \text{ AU/yr})$

HW7-7 Kepler x0= 1.0, vy0= 2.5π



Parabolic (Escape) Orbit

Initial position / velocity

$(x_0, y_0) = (1\ AU, 0)$

$(V_{x0}, V_{y0}) = (0, 2.8\pi\ AU/yr)$

At 8 AU
(8 x Earth-Sun distance); we stop program.