Numerical Approximations to Solutions of DEs

e.g. Time-independent Schrödinger Equation in one dimension.

Function: $\Psi(x)$
variable: x

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

order: 2
linear: ✓
homogeneous ✓

Quantum Harmonic Oscillator

$$V(x) = \frac{m}{2}\omega^2 x^2$$

$$-\frac{\hbar^2}{2m}\Psi''(x) + \frac{m}{2}\omega^2 x^2 \Psi(x) = E\Psi(x)$$

Problem: $[V(x)] = [E] = \frac{L^2 M}{T^2}$, $[x] = L$, $[m] = M$

$[\hbar] = \frac{L^2 M}{T}$, etc

Everything must be a dimensionless number for computation: Need to non-dimensionalize.

Define: dimensionless variable $u = \frac{x}{l_0}$

where l_0 is a constant length.

$\Rightarrow x = u\, l_0$, $dx = du\, l_0$

S.E. $$-\frac{\hbar^2}{2m}\frac{d^2 f(u)}{l_0^2\, du^2} + \frac{m}{2}\omega^2 l_0^2 u^2 f(u) = E f(u)$$

$$f''_{(u)} - \frac{m^2\omega^2 l_0^4}{\hbar^2} u^2 f(u) = -\frac{2m l_0^2 E}{\hbar^2} f(u)$$

Choose: $$l_0 = \sqrt{\frac{\hbar}{m\omega}}$$

$$f''_{(u)} - u^2 f(u) = -\frac{E f(u)}{(\frac{1}{2}\hbar\omega)} \equiv -\epsilon f(u)$$

$$\epsilon \equiv \frac{E}{(\frac{1}{2}\hbar\omega)} \leftarrow \text{dimensionless}$$

$$f''_{(u)} - (u^2 - \epsilon) f(u) = 0$$

f, u, ϵ all dimensionless

(Forward) Euler Method a.k.a. First-Order Runge-Kutta RK1

↳ problem: unstable

↳ error $\propto h^2$

solution: backward Euler Method

use the right side of interval.

other methods: Second-Order RK2

↳ error $\propto h^3$

Fourth-Order RK4

↳ error $\propto h^5$

Express our 2nd-order D.E. as a pair of coupled first-order DEs.

$y_1 = f$	$y_2 = f' = \frac{df}{du}$
$y_1' = f' \equiv y_2$	$y_2' = f'' = \frac{d^2f}{du^2} = (u^2 - \epsilon)\, y_1$

$f(u)$

Taylor expansion: Expand a function $g(x)$ around $x = k = x_0$

usually:

$$g(x) = \frac{g(k)}{0!} + \left.\frac{dg}{dx}\right|_{x=k} \frac{1}{1!}(x-k) + \frac{1}{2!}\left.\frac{d^2g}{dx^2}\right|_{x=k} (x-k)^2 \ldots$$

increment form:

$$g(x+h) = \frac{g(x)}{0!} + \frac{h}{1!}\frac{dg}{dx} + \frac{1}{2!} h^2 \frac{d^2g}{dx^2} + \ldots$$

$$\begin{cases} f(u+h) = f(u) + h\frac{df}{du} + \ldots \\ f'(u+h) = f'(u) + h\frac{d^2f}{du^2} + \ldots \end{cases}$$

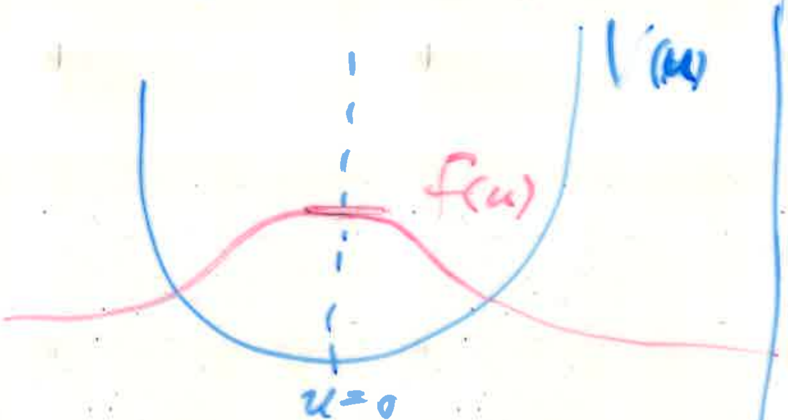
$$\begin{cases} y_1(u+h) = y_1(u) + h\, y_2(u) \\ y_2(u+h) = y_2(u) + h\,(u^2 - \epsilon)\, y_1(u) \end{cases}$$

Initial Conditions (Boundary Conditions)
at $u = 0$

<u>even</u>

$y_1 = 1$ (say)

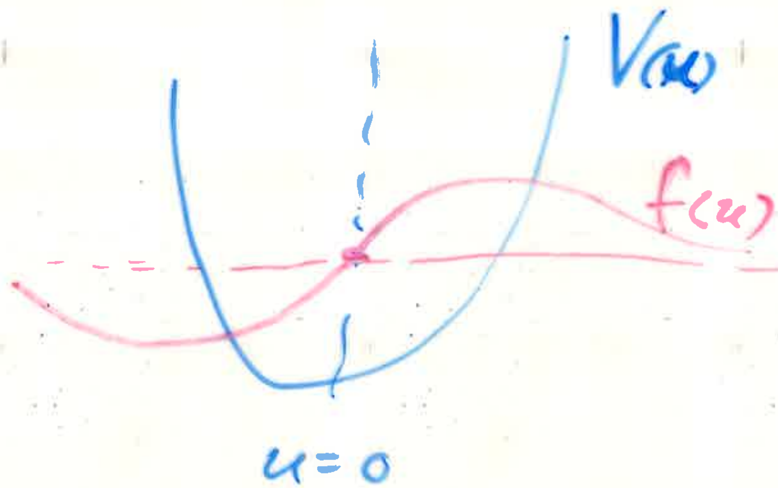
$y_2 = 0 = \frac{df}{du}$



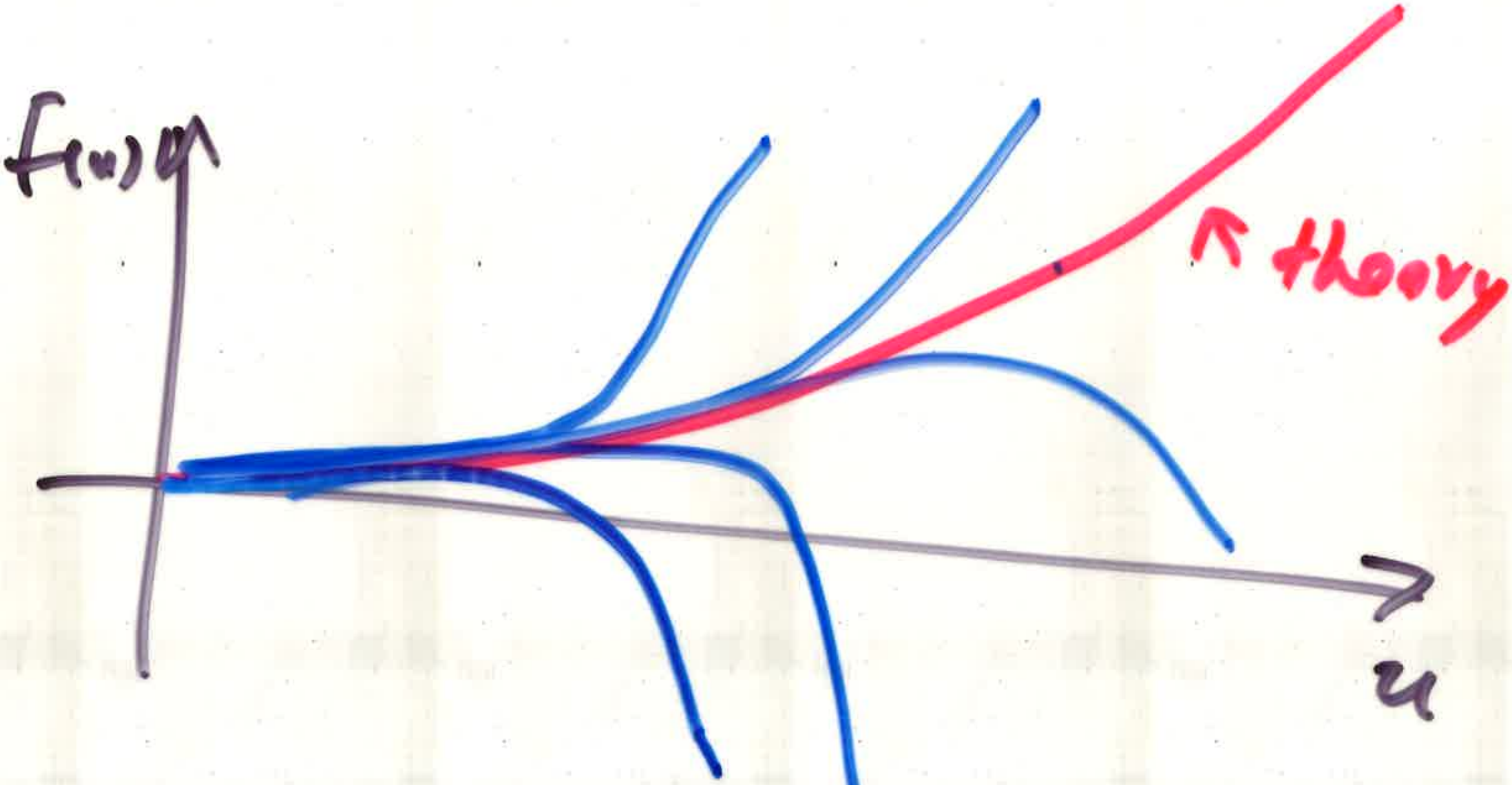
<u>odd</u>

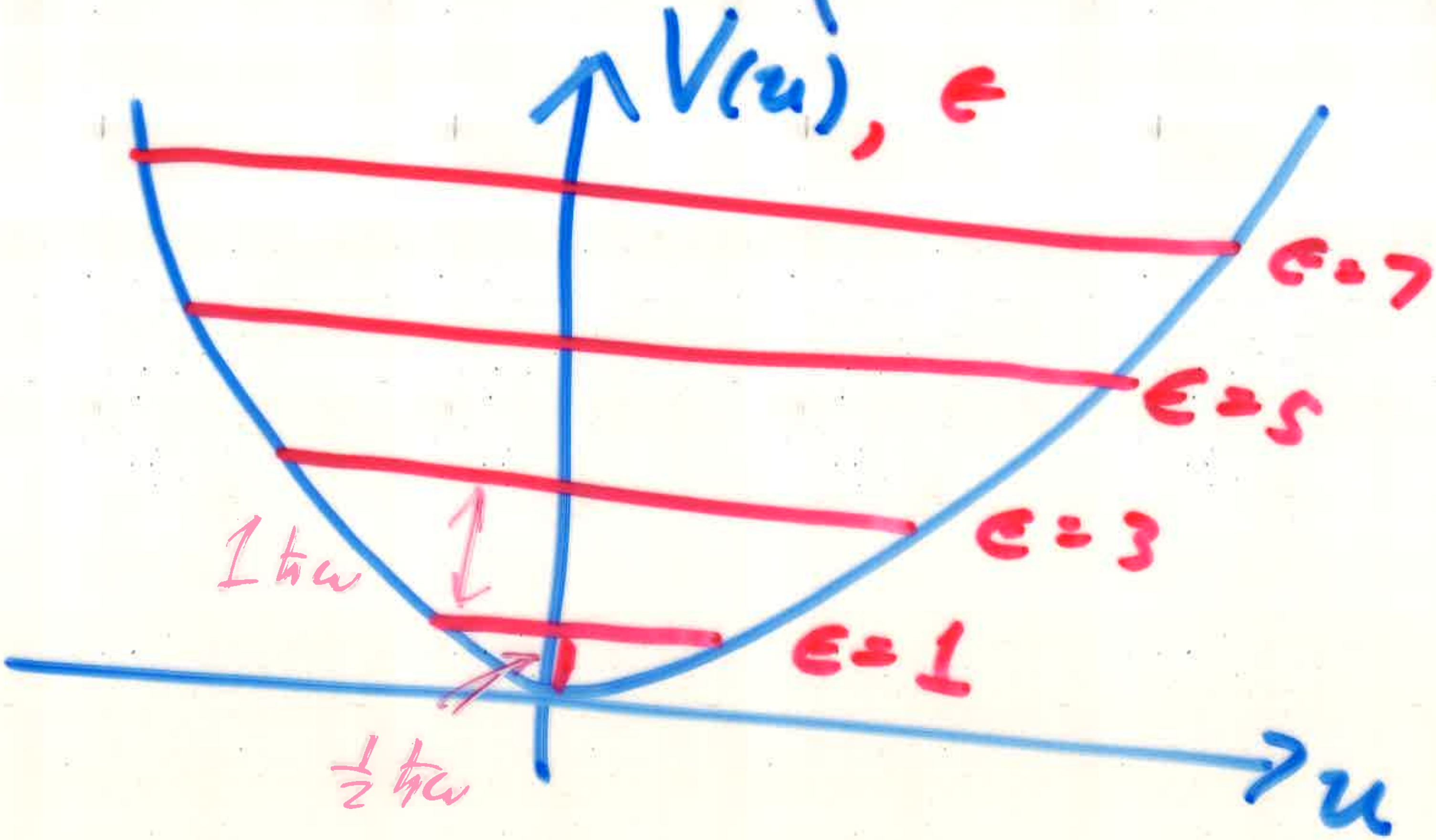
$y_1 = 0$

$y_2 = 1$ (say)



e.g. If want $f(u)$ between $u=0$, $u=10$
Stepsize $h = 0.01$, $N = 1000$


f(u)
theory
u


V(u), ε
ε=7
ε=5
ε=3
1ħω
ε=1
½ħω
u