First-order (forward) Euler — RK1

RK2

RK4

Express an equation as a pair of 1^{st} order differential equations.

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

Aside: Taylor series

$$g(x+h) = g(x) + h\frac{dg}{dx} + \ldots$$

$$f(u+h) = f(u) + h\frac{df}{du} + \ldots$$

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

$$y_1(u+h) \cong y_1(u) + h\,y_2(u)$$

$$y_2(u+h) \cong y_2(u) + h\,(u^2 - \epsilon)\,y_1(u)$$

If $f(x)$ has energy eigenvalue E

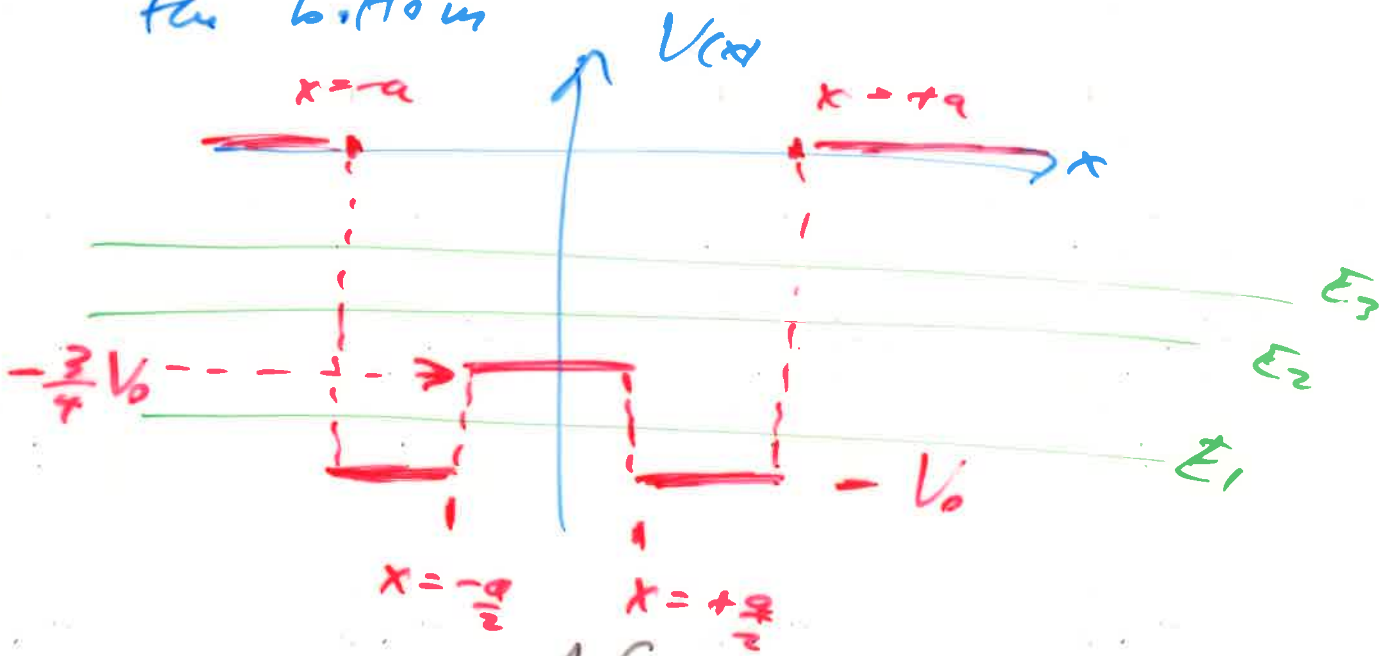
so does $2f(x)$.

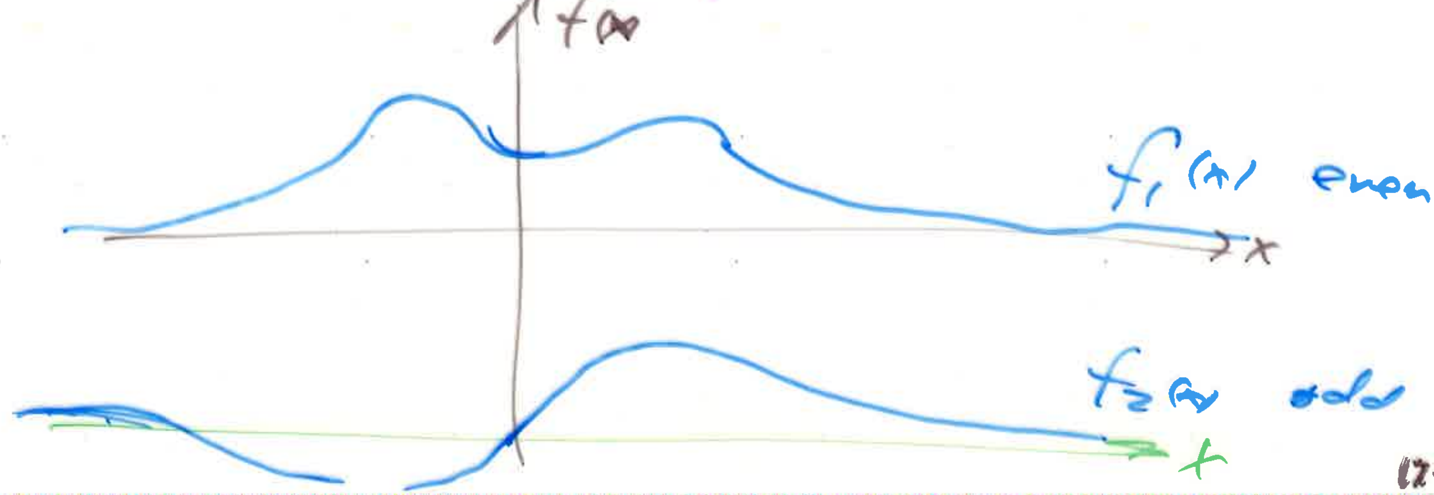
$$-\frac{\hbar^2}{2m} f''(x) + V(x) f(x) = E f(x)$$

Initial Conditions — at $x=0$

even solution	odd solution
choose $y_1 = 1$ (say)	$y_1 = 0$
$y_2 = 0$	$y_2 = 1$ (say)

Finite Square Well with a bump in the bottom





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

Need $V(x)$, $0 \le x \le \infty$ in functional form

Use Heaviside function

$$H(x) = \begin{cases} 0, & x<0 \\ 1, & x>0 \end{cases} \qquad H(0) \equiv \tfrac{1}{2} \checkmark$$

$$V(x) = -\tfrac{3}{4}V_0 H(x) - \tfrac{1}{4}V_0 H(x-\tfrac{a}{2}) + V_0 H(x-a)$$

$u \equiv \frac{x}{a}$ $\qquad x = ua \qquad dx = du\, a$

$$-\frac{\hbar^2}{2m}\frac{d^2 f(u)}{a^2 du^2} + V(x) f(x) = E f(x)$$

$$\frac{d^2 f(u)}{du^2} - \frac{2ma^2 V(u)}{\hbar^2} f(u) = -\left(\frac{2ma^2}{\hbar^2}\right) E f(u)$$

Define $\epsilon = \dfrac{E}{\left(\frac{\hbar^2}{2ma^2}\right)}$

Define $v = \dfrac{V_0}{\left(\frac{\hbar^2}{2ma^2}\right)} > 0$

$\Big\}$ dimensionless

Dimensionslosr
SE:

$$f''(u) + \frac{v}{4}\left[3\,\cancelto{1}{H(u)} + H(u-\tfrac{1}{2}) - 4\,H(u-1)\right] f(u) =$$
$$= -\epsilon\, f(u)$$

$$f''(u) + \left\{\frac{v}{4}\left[3H(u) + H(u-\tfrac{1}{2}) - 4H(u-1)\right] + \epsilon\right\} f(u) = 0$$

$$y_1 = f \qquad\qquad y_2' = f'' = -\frac{v}{4}\left\{3 + H(u-\tfrac{1}{2}) - 4H(u-1)\right] + \epsilon\right\} y_1$$

$$y_2 = y_1' = f'$$