MA3514 Test Solutions

1. let $\vec{y} = \begin{bmatrix} y \\ y' \end{bmatrix}$

$$\Rightarrow \frac{d\vec{y}}{dt} = \begin{bmatrix} y' \\ -(1+2t)y \end{bmatrix} = \vec{f}(t, \vec{y})$$

$$\vec{y}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \vec{y}_1 = \begin{bmatrix} y_1 \\ y_1' \end{bmatrix}$$

$$\Rightarrow \frac{\vec{y}_1 - \vec{y}_0}{h} = f\left(t_0 + \frac{h}{2}, \frac{1}{2}(\vec{y}_0 + \vec{y}_1)\right)$$

$$= f\left(0.05, \frac{1}{2}\begin{bmatrix} 1+y_1 \\ y_1' \end{bmatrix}\right)$$

$$= \begin{bmatrix} \frac{1}{2} y_1' \\ -(1+0.1)\frac{1+y_1}{2} \end{bmatrix} = \begin{bmatrix} 0.5 y_1' \\ -0.55 - 0.55 y_1 \end{bmatrix}$$

$$= \frac{1}{0.1} \begin{bmatrix} y_1 - 1 \\ y_1' \end{bmatrix}$$

$$\Rightarrow \quad y_1 - 1 = 0.05 y_1'$$

$$y_1' = -0.055 - 0.055 y_1$$

$$\Rightarrow: \begin{cases} y_1 - 0.05 y_1' = 1 \\ 0.055 y_1 + y_1' = -0.055 \end{cases}$$

$$\Rightarrow: \begin{cases} y_1 = 0.99452 \\ y_1' \approx -0.10970 \end{cases}$$

2. $T_{j+1} = y(t_j+h) + \frac{1}{4} y(t_j) - \frac{1}{2} y(t_j-h) - \frac{3}{4} y(t_j-2h)$
$- \frac{h}{8}\left[19 y'(t_j) + 5 y'(t_j-h)\right]$

$= y + hy' + \frac{h^2}{2} y'' + \frac{h^3}{6} y''' + \cdots$
$+ \frac{1}{4} y$
$- \frac{1}{2}\left[y - hy' + \frac{h^2}{2} y'' - \frac{h^3}{6} y''' + \cdots\right]$
$- \frac{3}{4}\left[y - 2hy' + 2h^2 y'' - \frac{8}{6} h^3 y''' + \cdots\right]$
$- \frac{h}{8}\left[19 y' + 5(y' - hy'' + \frac{h^2}{2} y''' + \cdots)\right]$

$= -\frac{5}{8} h^2 y''(t_j) + \cdots$

$\Rightarrow$ order $= 1$.

$1 + \frac{1}{4} - \frac{1}{2} - \frac{3}{4}$
$= \frac{5}{4} - \frac{2}{4} - \frac{3}{4} = 0$
$1 + \frac{1}{2} + \frac{3}{2} - \frac{24}{8} = 0$
$\frac{1}{2} - \frac{1}{4} - \frac{3}{2} + \frac{5}{8}$
$= -\frac{5}{4} + \frac{5}{8} = -\frac{5}{8}$

For zero-stability

let: $y_j = \lambda^j$

$\Rightarrow \lambda^3 + \frac{1}{4}\lambda^2 - \frac{1}{2}\lambda - \frac{3}{4} = 0$

factor it: $\lambda^3 - \lambda^2 + \frac{5}{4}\lambda^2 - \frac{5}{4}\lambda + \frac{3}{4}\lambda - \frac{3}{4} = 0$

$\Rightarrow \left(\lambda^2 + \frac{5}{4}\lambda + \frac{3}{4}\right)(\lambda - 1) = 0$

$$\Rightarrow \lambda_1 = 1 \qquad \lambda_{2,3} = \frac{-5 \pm \sqrt{23}\, i}{8}$$

$$|\lambda_{2,3}|^2 = \frac{1}{64}\left[25 + 23\right] = \frac{48}{64} < 1$$

zero-

$\Rightarrow$ Stable !

3. We define the I.V.P:

$$\begin{cases} y'' + y = x\,(y')^2, & x > 0 \\ y(0) = 1 \\ y'(0) = t \end{cases}$$

and $\phi(t) = y'(1) - \cdots t$

$\phi(t)$ can be obtained by solving the I.V.P for each given t.

Now for $\phi'(t)$: let

$$V = \frac{\partial y}{\partial t}$$

$$\Rightarrow: \begin{cases} V'' + V = 2x\, y' \cdot V' \\ V(0) = 0 \\ V'(0) = 1 \end{cases} \qquad \text{then: } \phi' = V'(1) - 1$$

We can solve y and V together to get ϕ, ϕ'.

4. (a). $y(t) = e^{iat}$,

(b). $y' = iay = f(t,y)$

$k_1 = f(t_j, y_j) = iay_j$

$k_2 = f(t_j + \frac{h}{2}, y_j + \frac{h}{2}k_1) = ia(y_j + \frac{h}{2}ia \cdot y_j)$

$= ia(1 + \frac{iah}{2})y_j$

$y_{j+1} = y_j + hk_2$

$= y_j + iah(1 + \frac{iah}{2})y_j$

$= \left[1 + iah + \frac{(iah)^2}{2}\right]y_j$

$\Rightarrow \left|1 + iah + \frac{(iah)^2}{2}\right|^2$

$= \left|1 - \frac{a^2h^2}{2} + iah\right|^2$

$= (1 - \frac{a^2h^2}{2})^2 + a^2h^2$

$= 1 - a^2h^2 + \frac{a^4h^4}{4} + a^2h^2$

$= 1 + \frac{1}{4}a^4h^4 > 1$

for fixed $h > 0$, $a \neq 0$

$\Rightarrow |y_j| \to \infty$ as $j \to \infty$

(c). If the x interval is truncated to (a, b) with a zero boundary condition, and x is discretized as

$$a = x_0, x_1, \cdots, x_n, x_{n+1} = b, \quad \text{where } x_j = x_{j-1} + \Delta x$$

then the Schrödinger equation is approximated by:

$$i\hbar \frac{du_j}{dt} = -\frac{\hbar^2}{2m} \cdot \frac{1}{(\Delta x)^2} \left[u_{j-1} - 2u_j + u_{j+1} \right] + V(x_j) u_j$$

$$\text{for } 1 \leq j \leq n$$

and
$$u_0 = 0, \quad u_{n+1} = 0 \qquad \text{where } u_j \approx u(x_j, t).$$

This gives rise to:

$$\frac{d}{dt} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} = iA \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} \quad \cdots\cdots (1)$$

where A is a real symmetric matrix.

It is known that a real symmetric matrix has only real eigenvalues: $\lambda_1, \lambda_2, \cdots, \lambda_n$. Let v_j be the eigenvector corresponding to λ_j, i.e. $Av_j = \lambda_j v_j$.

then. $v_j^T A = \lambda_j v_j^T$, (since $A^T = A$)

let $W_j = V_j^T \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}$

then if we multiply Eq. ① by V_j^T, we get.

$$\frac{d}{dt} W_j = i \lambda_j W_j \qquad \cdots\cdots ②$$

$$j = 1, 2, \cdots, n$$

In summary, the system of ODEs in Eq. ① is equivalent to uncoupled ODEs in Eq. ②. According to part (b), if the midpoint method is applied to Eq. ②, the numerical solution blows up, while the analytic solution remains bounded. Therefore, the numerical solution by midpoint method for the Schrödinger eq. will not be accurate.

Remark: You do not need to give such a detailed solution for the test, but it's better to give the main ideas.