DEPARTMENT OF MATHEMATICAL SCIENCES

COURSEWORK COVER SHEET

To be completed by the student

STUDENT(S)....Harry Lyness..

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DEPARTMENT: ....Mathematics...

DEGREE AND YEAR: ....MMath Mathematics, Year 3.......................................

LECTURER: Pranav Singh ....

UNIT CODE: MA40171 ....

TITLE OF ASSIGNMENT: ......MA40171 Assessed Coursework 1 — 2022/23..........

Declaration: "I certify that I have read and understood the entry in the Degree Courses Handbook for the Department of Mathematical Sciences on Cheating and Plagiarism and that all material in this assignment is my own work, except where I have indicated with appropriate references. I agree that, in line with Regulation 8.3, if requested I will submit an electronic copy of this work for submission to a Plagiarism Detection Service for quality assurance purposes."

Signature: Harry Lyness

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A particular form of plagiarism (and hence cheating) is auto-plagiarism or self-plagiarism. This occurs when a student submits work (whether a whole piece or part of a piece) without acknowledging that they have used this material for a previous assessment.

If you use someone else's work – say, by summarising it or quoting from it – you must reference the original author. This applies to all types of material – not only text, but also diagrams, maps, tables, charts, and so on. Be sure to use quotation marks when quoting from any source (whether original or secondary). Fully reference not only quotations, but also paraphrases and summaries. Such references should then be included in a bibliography or reference list at the end of the piece of work. Note that the need for referencing also applies to web-based material; appropriate references, including URLs, should always be given.

Further information on referencing work and plagiarism can be found on http://www.bath.ac.uk/keyskills (to be found under the sections on writing and IT skills).

Penalties for unfair practice will be determined by the Department or by the Faculty Board of Studies. They may include failure of the assessment unit or part of a degree, with no provision for reassessment or retrieval of that failure. Proven cases of plagiarism or cheating can also lead to an Inquiry Hearing or disciplinary proceedings.

Q1

a) $Q(\mathbf{v}) := \mathbf{v}^* H\mathbf{v}$ is real valued for any $\mathbf{v} \in \mathbb{C}^d$ if and only if $\mathbf{v}^* H\mathbf{v} = (\mathbf{v}^* H\mathbf{v})^*$. Using the relations $(AB)^* = B^* A^*$, $H = H^*$ and $(\mathbf{v}^*)^* = \mathbf{v}$,

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$$(\mathbf{v}^* H\mathbf{v})^* = (H\mathbf{v})^* (\mathbf{v}^*)^* = \mathbf{v}^* H^* (\mathbf{v}^*)^* = \mathbf{v}^* H\mathbf{v}$$

So, $\mathbf{v}^* H\mathbf{v} = (\mathbf{v}^* H\mathbf{v})^*$. This implies that $Q(\mathbf{v}) := \mathbf{v}^* H\mathbf{v}$ is real valued for any $\mathbf{v} \in \mathbb{C}^d$

b) If $\mathbf{y}(t)$ is the solution of the system of ODEs

$$\frac{d\mathbf{y}(t)}{dt} = iH\mathbf{y}(t), \quad t \in \mathbb{R}\backslash\{0\} \quad \mathbf{y}(0) = \mathbf{y}_0 \in \mathbb{C}^d$$

Then $\mathbf{y}(t)^*$ is a solution to the system of ODEs

$$\left(\frac{d\mathbf{y}(t)}{dt}\right)^* = (iH\mathbf{y}(t))^*, \quad t \in \mathbb{R}\backslash\{0\} \quad (\mathbf{y}(0))^* = (\mathbf{y}_0)^*$$

1

Notice that $(iH\mathbf{y}(t))^* = (H\mathbf{y}(t))^* i^* = -i\mathbf{y}(t)^* H^*$. Choose $\mathbf{x}(t) = \mathbf{y}(t)^*$, and since $H^* = H$,

$$\frac{d\mathbf{x}(t)}{dt} = (iH\mathbf{y}(t))^* = -i\mathbf{x}(t)H \quad t \in \mathbb{R}\backslash\{0\} \quad \mathbf{x}(0) = \mathbf{y}_0^*$$

as required.

c) H is hermitian since $H^* = H$. By spectral theorem for hermitian matrices, H has d linearly independent eigenvectors v_j with corresponding eigenvalues λ_j for $j \in \{1, ..., d\}$. There also exists a unitary matrix P such that $P^{-1}HP = D$, where $D = diag(\lambda_j)$, $P = [v_1, ..., v_d]$, and $D, P \in \mathbb{C}^{d\times d}$. Let $\mathbf{y}(t) = P\mathbf{z}(t)$.

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$$\frac{d\mathbf{y}(t)}{dt} = iH\mathbf{y}(t) \Rightarrow P\frac{d\mathbf{z}(t)}{dt} = iHP\mathbf{z}(t) \Rightarrow \frac{d\mathbf{z}(t)}{dt} = iD\mathbf{z}(t)$$

A j'th component of this is $z'(t) = i\lambda_j z(t)$ with general solution $z(t) = z(0)e^{i\lambda_j t}$. So, $||z(t)||_2 = ||z(0)||_2$ since $||e^{i\lambda_j t}||_2 = 1$. Notice that the linear transformation $\mathbf{y}(t) = V\mathbf{z}(t)$ preserves the solutions. This implies that $||\mathbf{y}(t)||_2 = ||\mathbf{y}(0)||_2$ for all $t \in \mathbb{R}_{\geq 0}$

d) Start by differentiating $Q(y(t))$.

1.5

$$\begin{aligned}
\frac{d(Q(\mathbf{y}(t)))}{dt} &= \frac{d}{dt}(\mathbf{y}^*(t)H\mathbf{y}(t)) \\
&= \frac{d\mathbf{y}^*(t)}{dt}H\mathbf{y}(t) + \mathbf{y}^*(t)H\frac{d\mathbf{y}(t)}{dt} \\
&= (-i\mathbf{y}^*(t)H)(H\mathbf{y}(t)) + \mathbf{y}^*(t)(HiH\mathbf{y}(t)) \\
&= i\mathbf{y}^*(t)HH\mathbf{y}(t) - i\mathbf{y}^*(t)HH\mathbf{y}(t) = 0
\end{aligned}$$

Hence $Q(\mathbf{y}(t)) = C$ for some $C \in \mathbb{R}$ for all $t \in \mathbb{R}_{\geq 0}$. Therefore $Q(\mathbf{y}(t)) = Q(\mathbf{y}(0))$

e) Differentiating $\mathbf{y}(t)$ using chain-rule, and noticing that $\frac{d\mathbf{y}_0}{dt} = 0$

$$\begin{aligned}
\frac{d\mathbf{y}(t)}{dt} &= \frac{d}{dt}(exp(itH))\mathbf{y}_0 + exp(itH)\frac{d\mathbf{y}_0}{dt} \\
&= iHexp(itH)\mathbf{y}_0 = iH\mathbf{y}(t)
\end{aligned}$$

As required

show

0.5

Q4

c)

1

- The most accurate method for conserving $||\mathbf{U}_N - \mathbf{y}(t)||_2$ is the LMM ($\clubsuit$) with $q = 4$ and $\beta_0 = 0.5$.
- The most accurate method for conserving $|\,||U_n||_2 - ||U_0||_2|$ is the trapezoidal rule, i.e. Adams–Moultons method for $q = 2$.

d)

The method which seems to conserve Q up to 10^{-15} is the trapezoidal rule, i.e. Adams–Moultons method for $q = 2$.

$$\mathbf{U}_{n+1} = \mathbf{U}_n + h\left(\frac{1}{2}\mathbf{f}_{n+1} + \frac{1}{2}\mathbf{f}_n\right)$$

To prove that this does conserve the value of Q, i.e. $Q(U_n) = Q(U_0)$, start by re-writing the trapezoidal rule using $\mathbf{f}_n = \mathbf{f}(\mathbf{U}_n) = iH\mathbf{U}_n$ and $\mathbf{f}_{n+1} = \mathbf{f}(\mathbf{U}_{n+1}) = iH\mathbf{U}_{n+1}$

$$\begin{aligned}
\mathbf{U}_{n+1} &= \mathbf{U}_n + \frac{h}{2}(iH\mathbf{U}_{n+1} + iH\mathbf{U}_n) \\
\mathbf{U}_{n+1} - \frac{h}{2}iH\mathbf{U}_{n+1} &= \mathbf{U}_n + \frac{h}{2}iH\mathbf{U}_n \\
\left(I - \frac{h}{2}iH\right)\mathbf{U}_{n+1} &= \left(I + \frac{h}{2}iH\right)\mathbf{U}_n \\
\mathbf{U}_{n+1} &= \left(I - \frac{h}{2}iH\right)^{-1}\left(I + \frac{h}{2}iH\right)\mathbf{U}_n
\end{aligned}$$

Since $f(A)g(A) = g(A)f(A)$,

$$\begin{aligned}
\mathbf{U}_{n+1} &= \left(I - \frac{h}{2}iH\right)^{-n}\left(I + \frac{h}{2}iH\right)^{n}\mathbf{U}_0 \\
Q(\mathbf{U}_{n+1}) &= \left(\left(I - \frac{h}{2}iH\right)^{-n}\left(I + \frac{h}{2}iH\right)^{n}\mathbf{U}_0\right)^{*} H\left(I - \frac{h}{2}iH\right)^{-n}\left(I + \frac{h}{2}iH\right)^{n}\mathbf{U}_0
\end{aligned}$$

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Then use $(A^*)^{-1} = (A^{-1})^*$

$$Q(\mathbf{U}_{n+1}) = \left(I + \frac{h}{2}iH\right)^{-n}\left(I - \frac{h}{2}iH\right)^{n}\mathbf{U}_0^{*}H\left(I - \frac{h}{2}iH\right)^{-n}\left(I + \frac{h}{2}iH\right)^{n}\mathbf{U}_0$$

Then apply $f(A)g(A) = g(A)f(A)$ again,

$$\begin{aligned}
Q(\mathbf{U}_{n+1}) &= \left(I - \frac{h}{2}iH\right)^{-n}\left(I - \frac{h}{2}iH\right)^{n}\left(I + \frac{h}{2}iH\right)^{-n}\left(I + \frac{h}{2}iH\right)^{n}\mathbf{U}_0^{*}H\mathbf{U}_0 \\
Q(\mathbf{U}_{n+1}) &= Q(\mathbf{U}_0)
\end{aligned}$$

Hence the trapezoidal rule conserves the value of Q.