Scienfic Computing Project 1

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Background Theory

The polarizability for a given frequency ω is obtained as a scalar product of two vectors **z** and **x**.

$$\alpha(\omega) = z^T x \tag{1}$$

z is obtained from the schrödinger equation and **x** is the solution to the following system of linear equation:

$$(E - \omega S)x = z \tag{2}$$

E and S are square matrices and ω is the frequency of the incoming light. E, S and z are visualized as follows:

$$E = \begin{bmatrix} A & B \\ B & A \end{bmatrix} \qquad S = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \qquad z = \begin{bmatrix} y \\ -y \end{bmatrix} \tag{3}$$

Question A

By computing the max-norm and the inverse of the given matrix we can calculate the condition number for the individual frequencies by using the following relation:

$$cond_\infty(M) = ||M||_\infty ||M^{-1}||_\infty \tag{4}$$

Frequencies	Condition Number
0.800	327.8167
1.146	152679.2687
1.400	227.1944

Tabel 1:

Question B

For the three frequencies we can also determine a bound on the relative forward error in the max-norm:

$$\frac{||\delta x||_\infty}{||\hat{x}||_\infty} \leq cond_\infty(E - \omega S) \frac{||\delta \omega S||_\infty}{||E - \omega S||_\infty} \tag{5}$$

Frequencies	Bound
0.800	0.0052
1.146	2.4050
1.400	0.0035

Tabel 2:

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