GX1974

OLLSCOIL na hÉIREANN, GAILLIMH

NATIONAL UNIVERSITY of IRELAND, GALWAY

WINTER EXAMINATIONS 2003

SECOND UNIVERSITY EXAMINATION

MATHEMATICS FOR MOLECULAR SCIENCE [MA 206]

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Time allowed: **Two** hours.
Full marks for **three** correct solutions.

1. (a) Define the terms **regular graph, connected graph** and **tree**. For the graphs given by the following adjacency matrices decide whether or not they are (i) connected, (ii) regular, (iii) trees:

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}; \; B = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(b) Consider the graph determined by the adjacency matrix A above, and let the function f take the constant value 1 on this graph. Show that the following eigenvector equation holds:

$$Af = 3f$$

(c) **Prove** that all the eigenvalues λ of A satisfy $|\lambda| \leq 3$.

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2. (a) List all trees on 6 vertices and on 7 vertices.
   (b) Prove that a saturated hydrocarbon with n carbon atoms has $2n+2$ hydrogen atoms.
   (c) Using part (a) or otherwise list all the **isomers** of C_7H_{16}.

3. (a) Define the **adjacency operator** A on complex–valued functions of a graph G.
   Prove that in the case of the Cayley graph $(Z_n, \pm 1)$ (the n–cycle), the adjacency operator A is a **convolution operator** i.e.:

$$Af = \delta_{\pm 1} * f$$

   where, in the usual notation

$$\delta_{\pm 1}(j) = \begin{cases} 1 & \text{if } j = \pm 1 \\ 0 & \text{otherwise} \end{cases}$$

   Hence by taking the *discrete Fourier transform* **prove** that the set of eigenvalues of A is given by

$$\left\{ 2\cos\frac{2\pi a}{n} \text{ such that } a = 0, 1, 2, \ldots, n-1 \right\}$$

   (b) Use part (a) to compute the rest mass energy $E = \frac{2}{n}\sum \lambda$, (where the sum is over the top $n/2$ eigenvalues of A), for benzene C_6H_6 and cyclobutadiene C_4H_4. Explain the significance of your answer in the context of Hückel theory.

4. (a) Let $\delta_{\pm 1}$ be as in Q3 (a), defined on the 5–cycle $(Z_5, \pm 1)$ and let f take the constant value b on $(Z_5, \pm 1)$. Calculate the following where $\widehat{f}$ or $\mathcal{F}f$ denotes the *discrete Fourier transform* of a function f, namely $(\mathcal{F}f)(x) := \sum_{y \in Z_5} f(y) e^{\frac{-2\pi i x y}{5}}$;

   (i) $\mathcal{F}f$, and $\mathcal{F}\delta_{\pm 1}$
   (ii) $\delta_{\pm 1} * f$.
   Verify that $\mathcal{F}(\delta_{\pm 1} * f) = \mathcal{F}\delta_{\pm 1} \cdot \mathcal{F}f$.

   (b) Suppose that $\Pi = \{z(0), z(1), \cdots, z(k-1)\}$ is the set of vertices of a closed polygon in the plane, with $k \geq 2$. Consider the so—called *(first) derived polygon*, say $\Pi^{(1)}$, obtained from Π by joining consecutively the mid–points of the sides of the original polygon, moving in an anti–clockwise sense.
   By iterating this procedure, the $m+$ 1st derived polygon $\Pi^{(m+1)}$ is obtained by joining the mid–points of the edges of the mth derived polygon $\Pi^{(m)}$.
   Give an outline of the use of the *discrete Fourier transform* to show that as $m \to \infty$, $\Pi^{(m)}$ approaches the *centroid* of the original polygon Π given by

$$\frac{z(0) + z(1) + \cdots + z(k-1)}{k}.$$

   (c) Draw a diagram of the process in part (b) to illustrate a polygon and the first three derived polygons.