Research Proposal

Characterisation of a connected graph whose energy does not exceed the number of vertices

Let G be a simple graph of order n, and let $\lambda 1, \lambda 2, \ldots, \lambda n$ be its eigenvalues (i.e., the eigenvalues of a (0,1)-adjacency matrix A(G) of G. Then the energy of G is defined as $E = E(G) = \sum_{i=1}^{n} |\lambda i|$. Consider the graphs satisfying the equation

$$E(G) \geq n \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

In 1973 the theoretical chemists published a paper in which they asked "why is the delocalization energy negative?". Translated into the language of graph spectral theory, their question reads: "why does the graph energy exceed the number of vertices?", understanding that the graph in question is "molecular". Recall that in connection with the chemical applications of E, a "molecular graph" means a connected graph in which there are no vertices of degree greater than three . What theoretical chemists failed to observe was that there exist "molecular" graphs violating the condition (1). These include acyclic graphs such as K1,2 and K1,3, with energies $2\sqrt{2} = 2.8284$ ... and $2\sqrt{3} = 3.4641$ ..., respectively. A less trivial example is the 7-vertex tree from Fig. 1, whose energy is $4 + 2\sqrt{2} = 6.8284$ ... Among graphs with cycles, the simplest such example is K2,3 for which $E = 2\sqrt{6} = 4.898979$ ... whereas n = 5. On the other hand, there are large classes of graphs ("molecular" or not) for which condition (1) is satisfied.

Result 1. If the graph G is non-singular (i.e., no eigenvalue of G is equal to zero), then (1) holds.

Result 2. If G is a graph with n vertices and m edges, and if $m \geq n^2/4$, then (1) holds

Result 3. If the graph G is regular of any non-zero degree, then (1) holds.

Problem Statements

Problem 1. Characterize the connected graphs for which Eq. (1) is not obeyed.

Problem 2. Characterize the connected graphs with $\Delta \leq k$ for which Eq. (1) is not obeyed, for k = 3, 4, 5,...

Problem 3. Characterize the trees with $\Delta \leq k$ k for which Eq. (1) is not obeyed, for k = 3, 4, 5,...