Molecular conduction and the characteristic polynomial

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The standard Hückel theory of conjugated hydrocarbons is equivalent to the problem of determining the spectrum of the adjacency matrix of the molecular graph. Conduction of an electron through a molecular electronic device is modelled by an extension of this theory. For conduction we solve the (now continuous) eigenvalue problem under the modified source-and-sink boundary conditions used by Ernzerhof and his group. It is found that the conductance varies strongly with the eigenvalue (representing the energy of the ballistic electron) but, within the approximations of Hückel theory, this property is fully determined by a combination of four characteristic polynomials: those of the molecular graph and three vertex-deleted sub-graphs. Trends and systematic descriptions of the physics to be expected from prototype molecular devices follow from this analytical expression. In particular, closed-form expressions and properties of the conductance function are deduced for some classes of chemical graphs. Relations of these ballistic currents to the 'ring currents' induced in aromatic molecules by magnetic fields will also be discussed.

Keywords: chemical graphs; adjacency matrices; eigenvalues; characteristic polynomials