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Extending transfer-matrix studies of charge transport in dsDNA: diagonal ladder model STEPHEN WELLS, RUDOPH ROEMER, University of Warwick — The π-stacking of aromatic bases along the axis of the DNA double helix suggests that DNA should be capable of supporting electron transport. This possibility has been investigated by a variety of experimental methods, including charge-transfer between intercalated dye molecules and direct measurement of conductivity in DNA molecules bridging two electrodes. In order to explore either the biological or nanotechnological significance of charge transport in DNA, we need theoretical models capable of predicting the influence of DNA sequence and structure on its charge transport properties. Transfer matrix methods have been used in conjunction with a ladder model of dsDNA (incorporating charge transfer between adjacent bases along a strand, and between hydrogen-bonded base pairs) to predict different transport properties for random, repetitive, or coding DNA sequences. It has been suggested that DNA charge transport may be involved in cellular mechanisms to detect and repair damage to DNA strands. We present extensions to the ladder model to allow for, firstly, charge transfer "diagonally" (from a base on a 5' strand to an adjacent base on a 3' strand, for example), and secondly, variations in hopping amplitudes due to bending of the helix (for example, in wrapping round a histone complex). Hence we take into account the extent of the electronic states and the geometry of the DNA strand in our modeling.

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