| Name-Surname | Haralampos Maroulis |
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| **Thesis Title** | *Charge transfer in one dimensional periodic DNA segments: tight binding method at the base pair level* |
| **Supervisor** | C. Simserides, Assistant Professor |
| **Summary** | We study simple carrier (hole or electron) transfer in some periodic B-DNA segments made up of N base pairs. We employ a Tight Binding approach at the base pair level using the on-site energies of the base pairs and the hopping integrals between successive base pairs. We assume that a carrier (hole or electron) is transferred through the HOMO or LUMO base pair's orbitals. At first, we study the time-independent problem by solving a system of N coupled differential equations and then we study the time-dependent problem by solving a system of N coupled first order differential equations. These Tight Binding parameters are taken from the literature. We study three types of periodic B-DNA segments, type α′, type β′ and type γ′, and for each of these we study the HOMO/LUMO eigenspectra, as well as the HOMO/LUMO densities of states (DOS). Then, we calculate the mean (over time) probabilities to find the extra carrier at each site (base pair) of a given segment, the Fourier spectra and other characteristic quantities of transport such as the pure mean transfer rates. Finally, we discuss the conclusions of charge transfer on those three types of B-DNA polymers. |
| **Key words** | DNA, tight binding, base pair, charge transfer, periodic B-DNA polymers |
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