Scrutinizing localization properties in heuristic models for DNA molecules: Localization lengths versus participation ratios

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Abstract

In this work we analyze the localization of electronic states of low-dimensional systems. We choose a well known strictly one-dimensional chain and an heuristic model for DNA-like molecules, in order to compare two established methods for analyzing the degree of localization, namely the localization length and participation ratio.

The potential applications of DNA in nanotechnology have attracted a great attention from different research communities. One of the leading questions is the possibility of building up nanoelectronics based on DNA, raising an even more fundamental question concerning the electronic properties of DNA and how to tune them [1]. In this scenario, another important point has proved to be relevant: the localization properties in these macromolecules. This involved question has to handle several problems, like the environment (wet or dry DNA), possible intra-chain correlations (sequencing), contacts and molecular structure (single versus double strands or even multiple helix chains). One aspect, the intrinsic base pairing, has been recently investigated [2] and the results, based on the wave function participation ratio (PR) (a measure of the fraction of the system sites over which the wave function is spread out), suggest that base pairing is a delocalization mechanism in the strict sense of enhancing the localization length (LL). This conclusion raised several criticisms that point to the conclusion that base pairing solely cannot promote a real delocalization [3].

A remarkable characteristic of the literature in the field is the lack of investigations comparing the different definitions of localization, hinting therefore the establishment of conclusive statements in some contexts, like the effect of base pairing on wave function extension in DNA. The aim of the present work is to compare the PR with the LL obtained from transmission probability calculations [3], $T(E) \propto \exp(-l/l_c)$, where $T(E)$ is the transmission probability at energy $E$, $l$ is the length of the chain and $l_c$ the LL. Initially we address a strictly one-dimensional system, the repulsive binary alloy, that shows truly delocalized states due to correlation in the disorder (a binary alloy with sites A and B, is said to be repulsive if B-like sites can have only A-like sites as first neighbors, while A-like ones can have both, A and B, as first neighbors) [4]. In Fig. 1 we compare both quantities, LL and PR, for a typical repulsive binary alloy [5]. One clearly observe that both definitions for the localization reveal the same properties of the system, pointing to a bona fide delocalized state near $E \approx -0.4$ eV. The PR clearly discloses a delocalization at a well defined peak structure. On the other hand, if the PR shows a smooth character, the scrutiny possibility of delocalization becomes less obvious.

This problem appears for the double chain case, Figs. 2 and 3, previously studied [2]. In Fig. 2 the single strand limit is depicted, for which no extended state is expected. Here both curves show a smooth character. In Fig. 3, both quantities also agree qualitatively. It should be mentioned,
however, that the chain length here is limited to only 35 base pairs. An important feature in scrutinizing the localization by means of the PR is the presence or absence of fluctuations. Smooth PRs indicate that the states are at least effectively delocalized \((l_c \gg l)\). An analysis of such fluctuations is also hindered for short chains.

A comparative scaling analysis for much longer chains for both, PR and LL, has still to be undertaken. The scaling for the PR for a DNA-like double chain has been partially presented in a previous work [2], but the transmission probabilities have to be looked carefully if one considers chains several thousand sites long. The double chain is the simplest multi-channel system and transmission probabilities obtained from traditional transfer matrices approaches may be precluded by subtle numerical instabilities [6]. Different approximations are sometimes used to overcome this instabilities [3], leading to another uncertainty in the comparison scenario. A systematic comparative study of different definitions of the localization of a state is a matter of future work.

References