Contents

Introduction **3**

1 DNA: a dynamical object **11**
1.1 An introduction to DNA 11
1.1.1 Structure of the DNA molecule: a helicoidal ladder 11
1.1.2 Functions of the DNA molecule: protein synthesis 14
1.1.3 Dynamics of the DNA molecule: transcription and denaturation processes 15
1.2 Transcription initiation processes and double helix structure. . . . 17
1.2.1 Transcription initiation process in details. DNA opening . 17
1.2.2 Observations and hypothesis for the dynamics of transcription activation 18
1.2.3 Structural deformation as the central feature for DNA opening 20
1.2.4 Supercoiling effects 21
1.3 Studying the transcription initiation by modeling DNA structure . 22

2 Modeling DNA structure: the *twist-opening* model **25**
2.1 Introduction 25
2.2 A planar model 28
2.2.1 The Peyrard Bishop model 28
2.2.2 The Multiple Scale Expansion solution of PB model 30
2.2.3 Thermal breathers as precursors for transcription 33
2.2.4 Effects of the specific DNA sequence 35
2.3 Motivations for the proposal of a new geometrical model 36
2.4 Presentation of the *twist-opening* model 38
2.4.1 Construction of the model 38
2.4.2 Some straightforward consequences on twist-opening coupling 42
2.5 Determination of the model constants 45
2.5.1 Morse potential parameters 46
2.5.2 The elastic constants 47
2.6 Dispersion relations for the model and rescaled Lagrangian 51
2.6.1 Rescaled approximate Lagrangian for small distortions . . 51

2.6.2 Dispersion relations . . . 53
2.7 Summary . . . 55

3 Analytical derivation of localized approximate solution in the *twist-opening* model 57
3.1 Looking for an extension of the PB breathers . . . 57
3.2 Multiple scale technique for multicomponent lattices . . . 58
3.2.1 The Multiple Scale Expansion technique . . . 58
3.2.2 Wave-packet in linear vectorial lattices . . . 60
3.2.3 Non Linear Vectorial Lattice . . . 64
3.3 Analytical small localized solutions for the *twist-opening* model . 68
3.3.1 Application of the multicomponent MSE technique to the model . . . 68
3.3.2 Envelope soliton approximate solutions . . . 73
3.4 Existence of solutions and parameter choice: PQ diagrams . . . 74
3.4.1 Small q breathers solutions of the model . . . 75
3.5 A "breathing" solution obtained with a different set of parameters 79
3.5.1 A small amplitude solution . . . 79
3.5.2 Solution with larger amplitude and limit of validity of the approximation . . . 84
3.6 First conclusions: acoustic solutions do not reproduce the "breathing" of DNA . . . 86
3.7 How to improve the model to recover oscillating breather solutions 88
3.7.1 A new stacking term . . . 88
3.7.2 Analytical solution on the optical branch . . . 90
3.7.3 Numerical simulation of the new solution . . . 93
3.8 Summary and conclusions . . . 95

4 Studies of thermal denaturation 97
4.1 Introduction . . . 97
4.2 The denaturation of DNA . . . 98
4.3 The simulation of the canonical ensemble with the Nosé Hoover method. . . . 99
4.4 Anharmonic stacking in the PB model . . . 103
4.5 Denaturation for the two versions of the *twist-opening* model with different values of G_0 . . . 105
4.5.1 Model without the direct stacking term W_{stack} . . . 105
4.5.2 "Breathing" in the improved *twist-opening* model . . . 112
4.5.3 Denaturation of the improved *twist-opening* model . . . 114

Conclusion 119

Appendices **123**
A The solution of the NLS equation 123
B The nonlinearity matrices of second ($c^{\nu}_{d,k}$) and third order ($C^{\nu}_{d,k,j}$) for the *twist-opening* model 125
C Coefficients for the correction terms and value of Q 126