行政院國家科學委員會補助專題研究計畫成果報告

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※　　軟態物質之物理及相關之彈性性質　　※
※　Physics of soft matter and related topics in elasticity　※
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計畫類別：o個別型計畫　　□整合型計畫
計畫編號：NSC　89－2112－M－032－032－(周子聰)
執行期間：89 年 11 月 1 日至 90 年 7 月 31 日

計畫主持人：　周子聰
共同主持人：

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□出席國際學術會議心得報告及發表之論文各一份
□國際合作研究計畫國外研究報告書一份

執行單位：淡江大學物理系

中　華　民　國　90 年 10 月 20　日

行政院國家科學委員會專題研究計畫成果報告

NSC Project Reports

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主持人：周子聰　　執行機構及單位名稱：淡江大學物理系
計畫參與人員：林方庭　執行機構及單位名稱：淡江大學物理系

一、中文摘要

雙股 DNA(double-stranded DNA, 即 dsDNA)分子的彈性性質與生物體的遺傳和演化有密切的關係。然而到目前為止尚未有一個模型能夠從微觀相互作用力的角度解釋 dsDNA 在所有外力和外力矩範圍內的異乎尋常的彈性性質。一個最近提出的模型(H. Zhou *et. al.*, Phys. Rev. Lett. 82, 4560 (1999), 即 ZZO 模型) 提供了這種可能性。我們用解析推導的方法論証了 ZZO 模型與熟知的棍狀蠕蟲鏈模型(wormlike rod chain model, 即 WLRC 模型)及拓廣的 WLRC 模型的關係。我們推導出了 ZZO 模型所對應的一組形態方程並用該方程組分析了 dsDNA 從 B 形態(B-form)到 S 形態轉變過程中的彈性性質及其相應形狀並得到與實驗相當符和的結果。我們也用類似的方法分析了 DNA 的蠕蟲鏈模型(WLC)的彈性性質及其相應形狀。我們還用計算機模擬的方法研究了雙股高份子鏈的彈性性質。

另一方面，盡管人們已對在通訊，生物，地質以及工程中有廣泛應用的網絡滲透模型做了大量研究，但仍然存在不少懸而未決的問題。我們用計算機模擬的方法研究了在外力作用下的隨機稀薄化(random diluted)的有心力網絡的臨界彈性性質。我們發現一個不太大的外力可以顯著地改變系統的臨界彈性性質。我們還發現其臨界指數並不隨外力的增長而單調,迅速地趨向隨機電阻(random resistor)網絡的相應臨界指數。

我們還發展了一對稱為固定切變系集(constant shear strain ensemble)的新的統計系集及該系集中的熱力學漲落公式。我們也推導出了等溫及絕熱彈性系數的最一般的"平衡漲落法"的計算公式，這些公式可望在計算機模擬材料性質中得到廣泛的應用。

關鍵詞：軟態物質，DNA 形態，彈性性質，無序網絡，滲透，統計力學

Abstract

The recent experiments have revealed that double-stranded DNA (dsDNA) has novel elastic property and its elasticity has very important biological significance. Therefore, a thorough investigation of the elasticity of dsDNA will enable us to gain better insight on many important biological processes concerned with life and growth. However, there is not yet a microscopic model to account for the fascinating elasticity of dsDNA in all range. A recently proposed model (H. Zhou, Y. Zhang, and Z.-C. Ou-Yang, Phys. Rev. Lett. **82**, 4560 (1999)) seems to be hopeful to provide a unified solution. We present an analytical based proof for the consistency between the ZZO model and the well accepted wormlike rod chain(WLRC) model as well as the generalized WLRC model. We investigate the abrupt extension of the contour length in the transition from the *B*-form to *S*-form of a dsDNA using ZZO model. Detail structural configurations are calculated and the results agree reasonably well with the experimental data. We also examine the classical mechanical solution of a WLC arbitrarily grafted at one end while stretching with an external force acting on the other end.

There are still many open questions on the rigidity of diluted networks after about three decades studies. We study the rigidity of a two dimensional site-diluted central force triangular networks under tension and at zero temperature. We calculate the shear modulus μ and find that the critical behavior of elasticity is sensitive to the stress. We also find that with increasing tension the critical concentrations of the systems decrease rapidly and monotonously into that of conductance of the random resistor network. However, the critical exponents of μ do no tend monotonously to that of conductance with increasing tension.

We develop the statistical mechanics of a pair of new ensembles called the constant shear strain ensemble. We present a direct calculation of thermodynamics properties for these new ensembles. We derive the general fluctuation expressions for both the isothermal and adiabatic elastic stiffness coefficients of systems with arbitrary inter-particle interactions and under arbitrary loading.

Keywords: soft matter, dsDNA conformations, elasticity, randomly diluted networks, percolation, statistical mechanics.

二、緣由與目的

As the genetic material, DNA molecule is of fundamental important in living organisms so that a thorough understanding of DNA molecule is a great challenge of our time. Despite definite progress made recently, our knowledge of DNA is still far from complete, especially in theoretical aspect concerning its conformations and deformations. DAN is a double-helical bio-polymer in which two chains of complementary nucleotides wind around a common axis to form a double-helical structure. Such a structure leads to mainly three kinds of deformations in double-stranded DNA(dsDNA): stretching and bending of the molecule, twisting of one nucleotide chain relative to its counterpart. The recent experiments revealed that dsDNA has novel elastic property. The relation between force and extension of a dsDNA molecule has clearly four elastic regimes for a torque-free dsDNA, and the applying of external torque adds more complexions to the elasticity of dsDNA. All these deformations have vital biological significance. Therefore, a thorough investigation of the elasticity of dsDNA will help us to gain better insight on many important biological processes concerned with life and growth. Concerning with one or another aspect of DNA elasticity, models were proposed and valuable insights were obtained. However, it is still a great challenge to understand systematically and quantitatively all aspects of dsDNA elasticity base on a unified framework. A typical open question is that what is the intrinsic reason i.e. what kind of interaction plays the vital role for dsDNA's elasticity, highly extensibility as well as its supercoiling property? We try to clarify this problem.

On the other hand, the percolation model has been a source of insight into many diverse areas of research, including communications, biology, physics, geophysics, and a host of engineering disciplines. Two important applications that commonly come to mind are those of fluid flow through porous media and the dc conductivity in a metal-insulator composite. It has also been employed to understand elasticity of tenuous media such as gels, sinters, glass or even biological networks of actin and other protein filaments *in vitro*. Therefore, to acquire a better insight of the mechanical property or the elasticity of a random diluted network is a very intrigue topic.

三、結果與討論：

1. We present an analytical based proof for the consistency between a new model, proposed by Zhou,

Zhang, and Ou-Yang (ZZO, Phys. Rev. Lett. **82**, 4560 (1999)), of the dsDNA and the well accepted wormlike rod chain(WLRC) model in the regime around the undistorted *B*-form. The relationship between the ZZO model and a recent proposed asymmetric elastic ribbon model is also discussed.

2. We develop the statistical mechanics of a pair of new ensembles called the constant shear strain ensemble that include the uniform dilation ensemble used frequently in computer simulations. We present a direct calculation of fluctuation formulae for the elastic constants, the specific heat and the thermal expansion tensor in these new ensembles.
3. We investigate the abrupt extension of the contour length in the transition from the *B*-form to *S*-form of a dsDNA under a stretching force in the framework of ZZO model. Using a classical mechanical approach, equations governing the structure of the dsDNA under external forces and torques are derived. The transition from the *B*-form to *S*-form can be understood in terms of an effective potential with a barrier separating these two states and resulting in a first-order transition. Detail structural configurations, such as loci of the two strands, relative extension, amount of self-untwisting and the threshold stretching force are calculated. Our results agree reasonably well with the observed experimental data.
4. Biomolecules, such as DNA, are often modeled by the Worm-Like Chain (WLC) model when pulled by an external force. We examine the classical mechanical solution of a WLC arbitrarily grafted at one end while stretching with an external force acting on the other end. Shape equations governing the configurations of the WLC are derived and chain configurations are solved numerically for arbitrary contour lengths and grafting conditions. Analytic results for the case of low force limit as well as near the fully stretched limit and long chain limit are also derived.
5. We derive the general fluctuation expressions for both the isothermal and adiabatic elastic stiffness coefficients of systems with arbitrary inter-particle interactions and under arbitrary loading.
6. We study the rigidity of a two dimensional site-diluted central force triangular networks under tension and at zero temperature. We calculate the shear modulus μ and find that the critical behavior of elasticity is sensitive to the stress. We also find that with increasing tension the critical concentrations (p*) of the systems decrease rapidly and monotonously into that of conductance of the random resistor network. However, the critical exponents *f*, by fitting into $\mu \sim (p-p^*)^f$, of μ do no tend monotonously to that of conductance with increasing tension.
7. We should say that there are still many open questions on the above topics so it will be worth for a further study.

四、計畫成果自評

原計畫研究 DNA **分子異乎尋常的彈性性質以及在外力作用下無序網絡的臨界彈性性質並預期在國際高水平的期刊上發表至少 4 篇文章．從第一部份,第三部份以及第五部份我們可以看到研究內容與原計畫基本相符並且稍有超出,因為固定切變系集和等溫及絕熱彈性系數的最一般的"平衡漲落法"的計算公式的推導並不在原計畫內。已發表的期刊論文加已投期刊的論文以及正在撰寫中的論文共有** 9 **篇，其中至少** 6 **篇發表在或投往/即將投往國際高水平的期刊上，超過預期目標。幾篇文章尚未完成的主要原因在於他們要求大量的計算機模擬時間,但由於經費到位較遲,未來得及配備好電腦因而延誤。由於同樣的原因,本計畫核定的消耗性器材費亦未用完。我們也必須指出由於這些課題的高度複雜性,在一年內完全解決這些問題是不可能的，因此非常值得進一步的探討。**

五、參考文獻：89 年 11 月 1 日至 90 年 7 月 31 日期間著述：

I. 已發表的期刊論文：

1．Z. Zhou(周子聰) and Pik-Yin Lai
"On the consistency of two elastic models for double-stranded DNA", Chem. Phys. Lett. (*accepted*).

2．周子聰
"DNA **的彈性性質**",**中華民國物理學會「物理雙月刊」**2001 **年** 8 **月號．**

3．Z. Zhou(周子聰)
"Fluctuations and thermodynamics properties of the constant shear strain ensemble", J. Chem. Phys. **114**, 8769(2001).

II. 國內研討會論文：

1. **Zicong Zhou(周子聰)** and Pik-Yin Lai**(黎璧賢)**
   "On the consistence of two elastic models for double-stranded DNA", 2001 **中華民國物理學會年匯暨研究成果發表會,**2001 **年二月十二日至** 2001 **年二月十四日，國立台灣大學物理系．**
2. **Zicong Zhou(周子聰)**
   "Fluctuations and thermodynamics properties of the constant shear strain ensemble"
   2001 **中華民國物理學會年匯暨研究成果發表會,**2001 **年二月十二日至** 2001 **年二月十四日，台北國立台灣大學物理系．**

III. 已投期刊的論文：

1. **Z. Zhou** and B. Joós
   "Fluctuation formulae for the elastic constants of an arbitrary system", *submitted to* Phys. Rev. B.
2. Pik-Yin Lai and **Z. Zhou**
   "Worm-Like Chain under an External Force: A Classical Mechanical Approach", *submitted to* Chinese Journal of Physics
3. Pik-Yin Lai and **Z. Zhou**
   "*B*-form to *S*-form Transition in a Double-stranded DNA", *submitted to* Phys. Rev. Lett.

IV. 正在撰寫中的論文：

1. **Z. Zhou**, B. Joós and Pik-Yin Lai
   "Elasticity of a stressed diluted network", *will be submitted to* Phys. Rev. Lett.
2. Pik-Yin Lai and **Z. Zhou**
   " B-form to S-form transition of a double-stranded DNA under a stretching force: A Classical Mechanical Approach", *will be submitted to* Phys. Rev. E.
3. Pik-Yin Lai and **Z. Zhou**
   "Structural properties of stretched double-stranded polymers: Twist and supercoil transitions"