



非線性動力系統之研究 III

Studies on Nonlinear Dynamical Systems III

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共同主持人：

- ☐赴國外出差或研習心得報告一份
- ☐赴大陸地區出差或研習心得報告一份
- ☒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

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一、 中文摘要

我們對於一種具有週期性位能，而且這些位能是由相同曲率的拋物線所組成的 Frenkel - Kontorova (FK)模型給出精確解。利用一組適當的相參數可以刻劃所有的具有環繞排序(rotationally ordered)的穩定結構，而這組相參數的元素可以進一步分解為次公度團(subcommensurate cluster)。過去先人在數值模擬所觀察到的隙結構(gap structure)的相變就對應到次公度團的分裂與結合，同時也就有非公度具有環繞排序的非再發(non-recurrent)穩定結構的產生。利用元相位移(elementary phase shift)的概念，可以分析出所有存在與基態簡併的穩定態的可能性，並且可以刻劃在相圖中所有的穩定域。在穩定域的邊界，非公度具有環繞排序的非再發穩定結構與基態簡併，

關鍵詞：

Abstract

We exactly solve a class of Frenkel-Kontorova (FK) models with a periodic potential composed of piece-wise convex parabolas having the same curvature. All rotationally ordered stable configurations can be depicted with appropriate phase parameters. The elements of a phase parameter are grouped into subcommensurate clusters. Phase transitions, manifested in the gap structure changes previously seen in numerical simulations, correspond to the splitting and merging of subcommensurate clusters with the appearance of incommensurate non-recurrent rotationally ordered stable configurations. Through the notion of elementary phase shifts, all the possibilities for the existence of configurations degenerate with the ground state are scrutinized and the domains of stability in the phase diagram are characterized. At the boundaries of a domain of stability, non-recurrent minimum energy configurations are degenerate with the ground state configurations and phase transitions occur.

Keywords: Frenkel-Kontorova model, commensurate-incommensurate phase transition, phase diagram, defect

二、 緣由與目的

Spatially modulated structures have been experimentally observed in many condensed matter physical systems[1]. The wave-vector characterizing the modulation varies with external parameters sometimes in a continuous manner but often remains constant, equal to a certain rational locking value, through some range of the external parameters. The physical origin of this complicated behavior is understood in terms of competing interactions in the free energy of the system. The FK class of models is one of the simplest among those models displaying such interesting behavior[2]. In this work, we will investigate a generalization of the "locking" behavior in a specific FK model and show that as the external parameters are adjusted to the boundary of the "locking" region, some "non-recurrent" configuration becomes degenerate with a recurrent one.

三、 結果與討論

We exactly solve an extension of the Aubry model, where the potential has d subwells in a period. This model was first proposed by Griffiths, et al[3]. Several interesting new phenomena such as the non-recurrent minimum energy (NRME) configuration in the incommensurate case, discontinuous cantor-cantor phase transitions (i.e., phase transitions in the gap structure), and independent orbits of gaps composing the complement of the CAM set (i.e., a gap structure with multiple *discontinuity classes* or *holes*[4] were found in the $d=2$ case. Recent work on this model[5,6] concentrated on acquiring ground state configurations through studying directional derivatives of the energy function, giving the average energy per atom, with respect to the elements in the phase parameter.

However, we establish that, for a given set of winding number and phase parameter, the depicted rotationally ordered (RO) configurations may *not be unique* up to shift operations. Thus the correspondence between RO configurations and phase parameters is not quite clear, and the meanings of the energy function as well as its derivatives for an arbitrary phase parameter are obsessed with ambiguity. Moreover, the above mentioned new phenomena found in the $d=2$ case have not been analyzed in the general case.

To resolve the ambiguity, we will provide two approaches. We first introduce the notion of subcommensurate clusters for the elements of a phase parameter. A phase parameter with multiple subcommensurate clusters builds up a composite hull function to describe a mixed phase. The meaning of the energy function on the whole space of phase parameters is thus clarified and the procedures adopted in [5,6] can be justified. Instead of studying the average energy per atom, another approach to determine if a given RO configuration is a ground state one is conducted through studying the energy differences resulting from moving some of the atoms across the potential tips. To keep the resultant configurations RO, we find that only a limited number (at most $2^d - 2$ for the case with d subwells in each period of potential) of such operations need be investigated. The evaluation of these energy differences is further reduced to solving a set of linear relations among some atomic positions.

The presence of multiple subcommensurate clusters in the phase parameter naturally leads to multiple compatible configurations (the mixed phase) in the commensurate case. To carry the notion of compatible configurations to the incommensurate case, we have to introduce the notion of extended numbers[7] as the elements in the phase parameter and then the non-recurrent RO (NRO) structure automatically emerges.

四、 計畫成果自評

In this work, we exactly solve a class of FK models, whose potential has d subwells in a period. The RO stable configuration is characterized by a winding number and a phase parameter with $d-1$ degrees of freedom. To depict *all* RO stable configurations with hull functions, phase parameters expressed in terms of extended numbers must be included for the incommensurate case. The depicted configurations in such cases are shown to be non-recurrent. The existence of these NRO configurations assures the existence of incommensurate NRME configurations for a suitable choice of potential parameters.

The notions of subcommensurate clusters, and resonance between different types of openings are introduced to fully characterize the gap structure. These notions are helpful in visualizing phase transitions in the gap structures.

We provided an approach to determine the ground state configurations through the

information about the relative positions of tips for the potential and gaps for the RO configurations. All the possibilities of degenerate ground state configurations are explored. Using these results, we are able to study the phase diagram. In the incommensurate case, we show that the phase diagram is an extension of the complete devil's staircase to $d-1$ dimensions. It will be interesting to see if the conclusion is still valid in the $d \rightarrow \infty$ limit.

We also provided a general method to implement an incommensurate NRME configuration. For any FK model beyond transition by breaking the analyticity, which allows more than one discontinuity classes, it appears that such incommensurate NRME configurations should also exist at the transition points for any l to $(l+1)$ -hole transitions. In general, NRME configurations emerge as long as a certain locking condition (either the subcommensurate condition in our case or the commensurate condition) of the parameters to characterize the configuration (including the phase parameters in our case and the winding number) is allowed to break down, which are expected to occur at boundaries of the domains of stability, where some locking conditions prevail.

五、 參考文獻

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