Vol 17 No 5, May 2008
1674-1056/2008/17(05)/1623-06

Chinese Physics B

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# Quantum phase transition and von Neumann entropy of quasiperiodic Hubbard chains*

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(Received 20 November 2007; revised manuscript received 24 December 2007)

The half-filled Hubbard chains with the Fibonacci and Harper modulating site potentials are studied in a self-consistent mean-field approximation. A new order parameter is introduced to describe a charge density order. We also calculate the von Neumann entropy of the ground state. The results show that the von Neumann entropy can identify a CDW/SDW (charge density wave/spin density wave) transition for quasiperiodic models.

**Keywords:** von Neumann entropy, quasiperiodicity, Hubbard model, spin-density waves
**PACC:** 0367, 6140M, 7110F, 7530F

## 1. Introduction

Since the discovery of quasicrystals and quasiperiodic superlattice in laboratory,[1−3] the electronic properties of quasicrystals have brought a great interest in recent condensed matter physics. The electronic states in such materials are not trivial even in the simplest case of one-dimensional free fermions. Meanwhile, the strongly correlated electronic system[4,5] has been an important subject in condensed matter physics especially since the discovery of high $T_c$ oxide superconductors and heavy fermion materials.[6−8] So the interplay between quasiperiodicity and strong correlation will be very interesting. However, most of previous studies focused on the effects of disorder and correlations[9−13] by using different methods,[14−19] and few studies have been carried out in the effects of quasiperiodicity and correlations.[20−22] The effect of electronic interaction on electronic properties of a quasiperiodic lattice can be studied by observing electronic distributions (using charge density wave (CDW) and spin density wave (SDW) parameters, etc); this effect has been studied in a periodic situation successfully. But for a quasiperiodic system, the usual CDW parameter for a uniform and periodic system is not a good charge order parameter.[22]

On the other hand, some evidences show that many problems involved in strongly coupled many-body systems can be characterized and classified by using quantum entanglement. Quantum entanglement, as one of the most intriguing features of quantum theory, has been a subject of many studies in recent years. In particular, whether there exists any relationship between entanglement and quantum phase transition in fermion systems is one of the most important issues.[23−27]

In view of this perspective we attempt to study the competition between quasiperiodicity and on-site electronic correlations for electrons in one dimension. In order to describe the distribution of charges in a quasiperiodic system, we introduce a new charge order parameter. The present study mainly concentrates on properties of ground state of half-filled one-dimensional Fibonacci and Harper modulating Hubbard chain by using a new charge order, spin density order and ground state von Neumann entropy (one popular measure of entanglement). And we reveal a relationship between the von Neumann entropy and the CDW–SDW transition.

The rest of this paper is organized as follows. In Section 2 we introduce two quasiperiodic Hubbard models: Fibonacci model and Harper model. The self-consistent Hartree–Fock approach (SCHFA) and the von Neumann entropy are briefly described in Section 3. In Section 4 we discuss the results obtained from the SCHFA and the von Neumann entropy. Given in

*Project supported by the National Natural Science Foundation of China (Grant Nos 90203009, 10175035 and 10674072), the Specialized Research Fund for the Doctoral Programme (SRFDP) of Higher Education of China (Grant No 20060319007), and the Foundation for outstanding Young Teacher of Ministry of Education of China.
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Section 5 are the conclusions drawn from the present study.

## 2. The model

We consider a finite chain of $N$ sites, given by the Hamiltonian

$$H = \sum_i \varepsilon_i(n_{i\uparrow}+n_{i\downarrow}) + U\sum_i n_{i\uparrow}n_{i\downarrow} - t\sum_{i,\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + c^\dagger_{i+1\sigma}c_{i\sigma}), \quad (1)$$

where the number operator $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$, $c^\dagger_{i\sigma}(c_{i\sigma})$ is the creation(annihilation) operator for an electron of spin $\sigma(=\uparrow,\downarrow)$ at the site $i$, $t$ is the hopping between nearest neighbouring sites, $U(>0)$ is the on-site Coulomb interaction, $\varepsilon_i$ is the site energy at the $i$th site. Here we study two kinds of most common quasiperiodic models: Fibonacci and Harper model.

### 2.1. Fibonacci Hubbard model

For a Fibonacci chain, $\varepsilon_i$ takes on $\varepsilon_A$ or $\varepsilon_B$ depending on the Fibonacci sequence. A usual way of introducing the Fibonacci sequence is to employ an inflation like procedure $B \to A$ and $A \to AB$. For instance, from seed $A$, we obtain the Fibonacci chain

$$ABAABABAABAABABAABABAABAABAB\cdots. \quad (2)$$

For an infinite Fibonacci chain, the ratio of $A$ to $B$ is $(\sqrt{5}+1)/2$, which is known as the golden mean. For $U=0$, Hamiltonian (1) describes a single particle Fibonacci model. The electronic states are critical and multifractal in this system.[28]

### 2.2. Harper Hubbard model

For the Harper model, the site-dependent potential is chosen to be $\varepsilon_i = \lambda\cos(2\pi\sigma i)$, where $\sigma = (\sqrt{5}-1)/2$. For $U=0$, Hamiltonian (1) describes the usual Harper model. The Harper model undergoes a metal–insulator transition at $\lambda=2$. For $\lambda<2$, all the states are extended; for $\lambda>2$, all the states are localized; for $\lambda=2$, all the states are critical.[29]

## 3. SCHFA method and von Neumann entropy

### 3.1. SCHFA method

Using the SCHFA the on-site $U$ term is modified as

$$Un_{i\uparrow}n_{i\downarrow} \simeq U\ (\ \langle n_{i\downarrow}\rangle n_{i\uparrow} + \langle n_{i\uparrow}\rangle n_{i\downarrow} - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle), \quad (3)$$

then the Hamiltonian is decoupled into up-spin and down-spin parts:

$$H = H_\uparrow + H_\downarrow - U\sum_i\ \langle n_{i\downarrow}\rangle\ \langle n_{i\uparrow}\rangle, \quad (4)$$

where

$$H_\uparrow = -t\sum_i\left(c^\dagger_{i\uparrow}c_{i+1\uparrow} + c^\dagger_{i+1\uparrow}c_{i\uparrow}\right) + \sum_i \varepsilon_i n_{i\uparrow} + U\sum_i\ \langle n_{i\downarrow}\rangle n_{i\uparrow}, \quad (5)$$

and

$$H_\downarrow = -t\sum_i\left(c^\dagger_{i\downarrow}c_{i+1\downarrow} + c^\dagger_{i+1\downarrow}c_{i\downarrow}\right) + \sum_i \varepsilon_i n_{i\downarrow} + U\sum_i\ \langle n_{i\uparrow}\rangle n_{i\downarrow}. \quad (6)$$

After we have obtained a self-consistent solution of Hamiltonian equation, we can have a distribution of electrons $n_{i\uparrow}, n_{i\downarrow}$ in a ground state. In this paper, we study only the half-filled case.

However, because of the quasiperiodicity, the distribution of particles is not uniform (see Fig.1). So according to a traditional definition of CDW parameter $C = \frac{1}{N}\sum_i (-1)^i\langle(n_{i\uparrow}+n_{i\downarrow})\rangle$, the value of CDW parameter is nearly zero (see Fig.2). Here we introduce a new charge order parameter instead of usual CDW order parameter, which is defined as:

$$C = \frac{1}{N}\sum_i\ g(i)\ \langle(n_{i\uparrow}+n_{i\downarrow})\rangle, \quad (7)$$

where $i = 1,\cdots,N$ label the sites of the chain. For the Fibonacci model, $g(i) = -1$ (1) if $\varepsilon_i$ belongs to $\varepsilon_A(\varepsilon_B)$ in the Fibonacci sequence. For the Harper model, $g(i) = \cos(2\pi\sigma i)$.

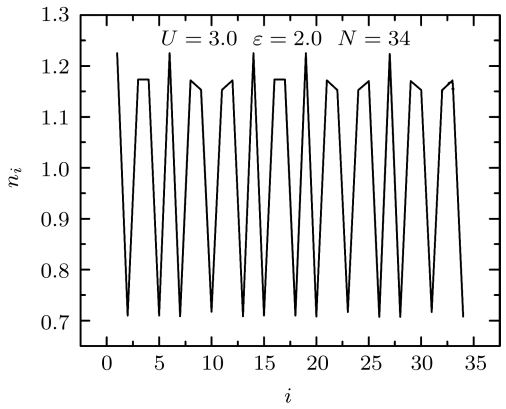



**Fig.1.** The particle density $n_i$ versus site $i$ for a Fibonacci Hubbard chain with $\varepsilon_B = 2.0$, $\varepsilon_A = 0.0$, and $N = 34$.

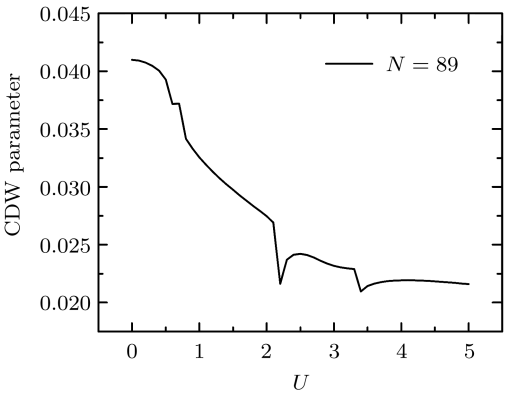



**Fig.2.** The CDW parameter versus $U$, with values of $\varepsilon_B = 2.0$ and $\varepsilon_A = 0.0$ in a Fibonacci Hubbard chain. The value of CDW parameter is nearly zero.

For the SDW parameter, we still take the traditional definition

$$S = \frac{1}{N}\sum_i (-1)^i \langle (n_{i\uparrow} - n_{i\downarrow})\rangle. \tag{8}$$

### 3.2. von Neumann entropy

For fermion systems, there are four possible local states at each site i.e. $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$. We consider a local density matrix of the ground state $|\Psi\rangle$, which is a reduced density matrix $\rho_i = \mathrm{Tr}_i|\Psi\rangle\langle\Psi|$, where $\mathrm{Tr}_i$ denotes tracing over all sites except the $i$th site. Accordingly, the von Neumann entropy $E^i_\nu$ calculated from the reduced density $\rho_i$ measures the entanglements of state on the $i$th site with those on the remaining $L-1$ sites. It is called the local entanglement, for it exhibits the correlations between a local state and the states of the other part of the system. The local density matrix $\rho_i$ is

$$\begin{aligned}\rho_i = {} & z_i\,|0\rangle\langle 0| \;+\; u_i^+\,|\uparrow\rangle\langle\uparrow| \;+\; u_i^-\,|\downarrow\rangle\langle\downarrow| \\ & + w_i\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow|,\end{aligned} \tag{9}$$

where

$$\begin{aligned} w_i &= \langle n_{i\uparrow} n_{i\downarrow}\rangle, \\ u_i^+ &= \langle n_{i\uparrow}\rangle - w_i, \\ u_i^- &= \langle n_{i\downarrow}\rangle - w_i, \end{aligned}$$

and

$$z_i = 1 - \langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle + w_i. \tag{10}$$

The corresponding von Neumann entropy is defined as

$$\begin{aligned} E^i_\nu = {} & -u_i^+ \log_2 u_i^+ - u_i^- \log_2 u_i^- \\ & - w_i \log_2 w_i - z_i \log_2 z_i. \end{aligned} \tag{11}$$

For nonuniform systems, the $E^i_\nu$ depends on site $i$. Therefore, we use the average value of von Neumann entropy without the loss of generality,[26] expressed as

$$\begin{aligned} E^e_\nu = {} & \frac{1}{N}\sum_i (-u_i^+ \log_2 u_i^+ - u_i^- \log_2 u_i^- \\ & - w_i \log_2 w_i - z_i \log_2 z_i). \end{aligned} \tag{12}$$

The entanglement is important for determining the physical properties of the system.[25]

## 4. The results of SCHFA calculations and von Neumann entropy

### 4.1. Fibonacci Hubbard model

For the Fibonacci Hubbard model at half filling, the value of new order parameter $C$ decreases with $U$ increasing (see Fig.3(a)). There is a turning point $U_c$, and the value of $C$ decreases more quickly after $U_c$. The turning point is confirmed by the SDW parameter, as shown in Fig.3(b). When $U < U_c$, the value of SDW parameter $S$ is almost zero; when $U > U_c$, the value of $S$ is not zero, and increases with $U$ increasing. The behaviours of $C$ and $S$ of the Fibonacci Hubbard model are similar to those of the periodic Hubbard model, but are different from those for a uniform model in which there exists no CDW state.[30]

The results indicate that because of competition between correlation and quasiperiodicity, when the value of $U$ is small compared with the value of $\varepsilon_B$–$\varepsilon_A$, it is a CDW state, in which the effect of quasiperiodicity is obvious and the particle density resembles a quasiperiodic modulation; when the value of $U$ is large compared with the value of $\varepsilon_B$–$\varepsilon_A$, it is an SDW state, in which the effect of $U$ is more obvious than the effect of quasiperiodicity and the spin density varies from site to site, but the particle density is still not uniform in distribution due to quasiperiodicity (see Fig.1).

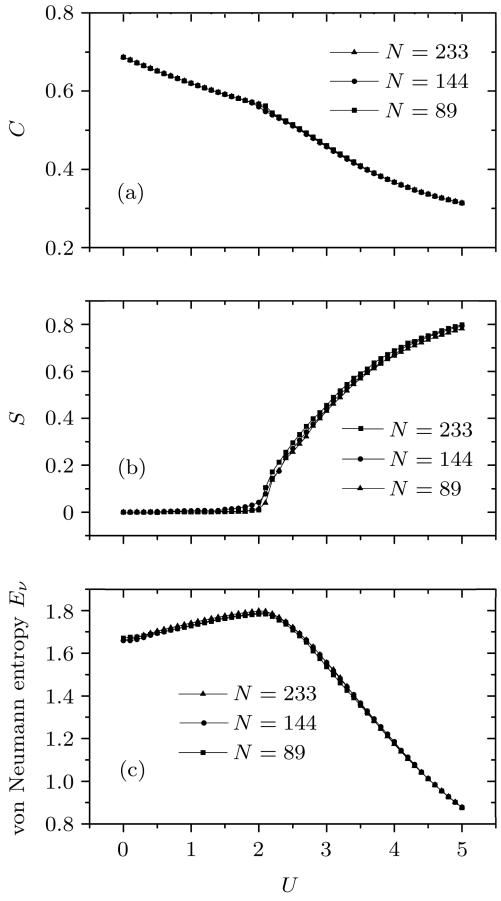



**Fig.3.** (a) The new charge order parameter $C$ versus $U$; (b) The SDW parameter $S$ versus $U$; (c) von Neumann entropy $E_\nu$ versus $U$. The three lines with different symbols are for Fibonacci Hubbard chains each with values of $N$ : 89, 144, and 233, $\varepsilon_B = 2.0$, and $\varepsilon_A = 0.0$.

In order to describe the CDW–SDW transition, we also use the von Neumann entropy to describe the quasiperiodic models. The von Neumann entropy has been used to study the quantum phase transition in the uniform Hubbard model and the extended Hubbard model successfully.[25] Here we use the von Neumann entropy to describe quasiperiodic models. We calculate the von Neumann entropy for Fibonacci Hubbard chains in Fig.3(c). The results show that there exists a maximum value of von Neumann entropy. The position of maximum value indicates a turning point, which is the same as that in a uniform system.[25] The turning point indicated by von Neumann entropy coincides with that indicated by $C$ and $S$. Therefore, we find that the von Neumann entropy is a useful quantity to identify the CDW–SDW transition in describing quasiperiodic models.

All these results are given in different sizes of chains, and they are nearly the same, which implies that the finite size effect is not significant here. And for different values of $\varepsilon_B - \varepsilon_A$, the results show similar behaviours. When the value of $\varepsilon_B - \varepsilon_A$ is large, the turning point $U_c$ indicated by $C$ is much more obvious (see Fig.4).

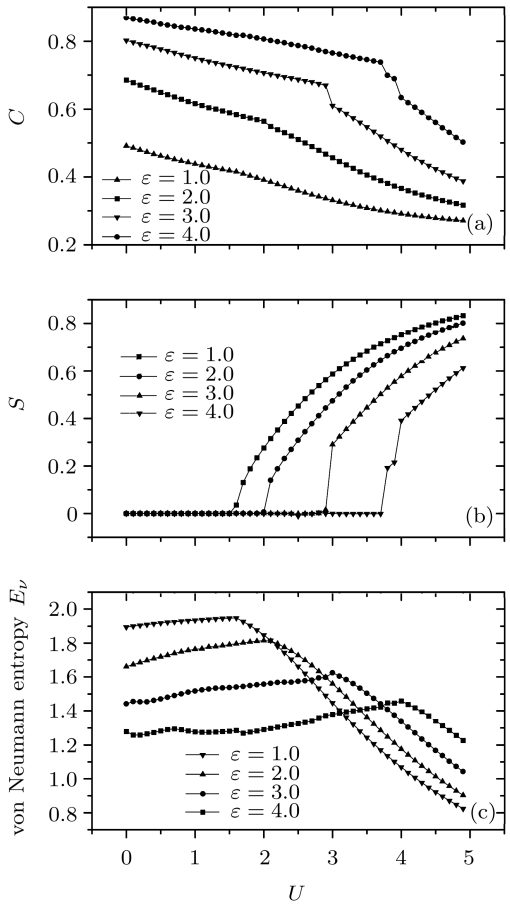



**Fig.4.** (a) The new charge order parameter $C$ versus $U$; (b) The SDW parameter $S$ versus $U$; (c) The von Neumann entropy $E_\nu$ versus $U$. The four lines with different symbols are for Fibonacci Hubbard chains ($N = 34$) each with values of $\varepsilon_B$ : 1.0, 2.0, 3.0, and 4.0.

## 4.2. Harper Hubbard model

For the Harper Hubbard model with half filling, we study the effects of $\lambda$ and $U$. For a usual Harper

model ($U = 0$), there exists a metal–insulator transition at $\lambda = 2.0$. When $\lambda < 2.0$, all electronic states are extended; when $\lambda > 2.0$, all electronic states are localized. Therefore, we study the effects of $U$ on two different value of $\lambda$ ($\lambda = 1.0$ and $\lambda = 4.0$) that represent $\lambda < 2.0$ and $\lambda > 2.0$ respectively (see Figs.5 and 6). Behaviours of $S$ and $C$ for $\lambda < 2.0$ are similar to those for $\lambda = 1.0$; behaviours of $S$ and $C$ for $\lambda > 2.0$ are similar to those for $\lambda = 4.0$. We find that for both

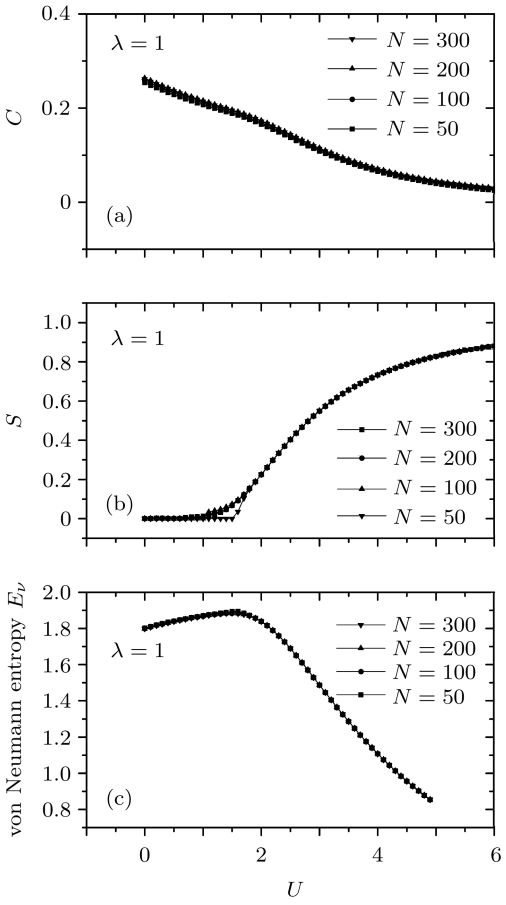



**Fig.5.** (a) The new charge order parameter $C$ versus $U$. (b) The SDW parameter $S$ versus $U$. (c)The von Neumann entropy $E_\nu$ versus $U$. The four lines with different symbols are for Harper Hubbard models each with the values of $N$ : 50, 100, 200, and 300, and $\lambda = 1.0$.

$\lambda < 2.0$ and $\lambda > 2.0$, there exists a turning point $U_c$ indicated by $C$ (see Figs.5(a) and 6(a)) and $S$ (see Figs.5(b) and 6(b)). For $\lambda < 2.0$, behaviours of $S$ and $C$ for the Harper Hubbard model are similar to those for the Fibonacci Hubbard model, and the system is more like a periodic system. But for $\lambda > 2.0$, when $U < U_c$ the behaviour of $S$ is different from that for $\lambda < 2.0$, and there appears an SDW state. The value of $S$ is not zero, there is a little increase in value of $S$.

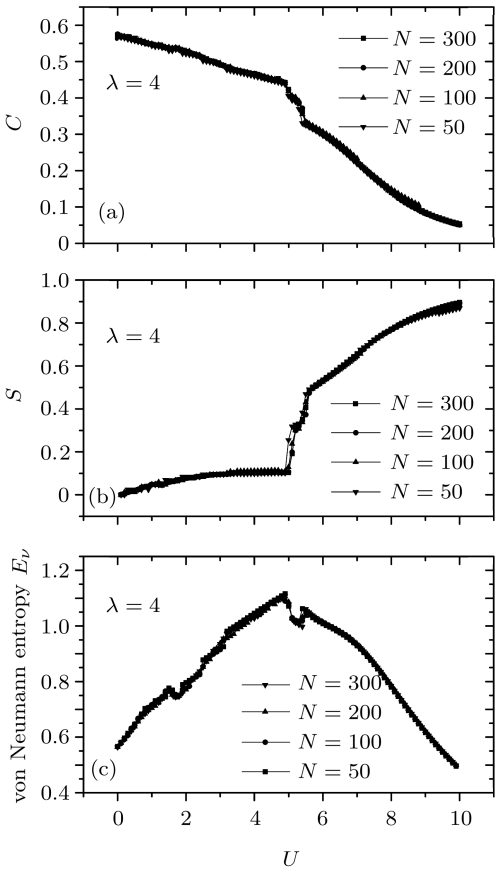



**Fig.6.** (a) The new charge order parameter $C$ versus $U$. (b) The SDW parameter $S$ versus $U$. (c) The von Neumann entropy $E_\nu$ versus $U$. The four lines with different symbols are for Harper Hubbard models each with the values of $N$ : 50, 100, 200, and 300, and $\lambda = 4.0$.

Because when $\lambda > 2.0$, all electronic states are localized states. There are more chances for two electrons with opposite spins to occupy the same site, which will induce a large value of $U$. But in fact the value of $U$ is small. Therefore, there must be a little stagger distribution of up-spin and down-spin for partial sites (see Fig.7). From this point of view, we obtain that when $\lambda > 2.0$, the SDW order for $U < U_c$ in the Harper Hubbard model is caused by the localization of electronic states.

Then we study the von Neumann entropy for the Harper Hubbard model. And the turning point $U_c$ is confirmed by the position of maximum value of von Neumann entropy (see Figs.5(c) and 6(c)).

From the above discussion, we find that for the Harper Hubbard chain, there exists still a turning point $U_c$ for the SDW–CDW transition. For $\lambda < 2.0$, the model is similar to the Fibonacci Hubbard model. But for $\lambda > 2.0$ the behaviour of $S$ is different because of localization of electronic stats, the value of $S$ is not zero even when $U < U_c$.

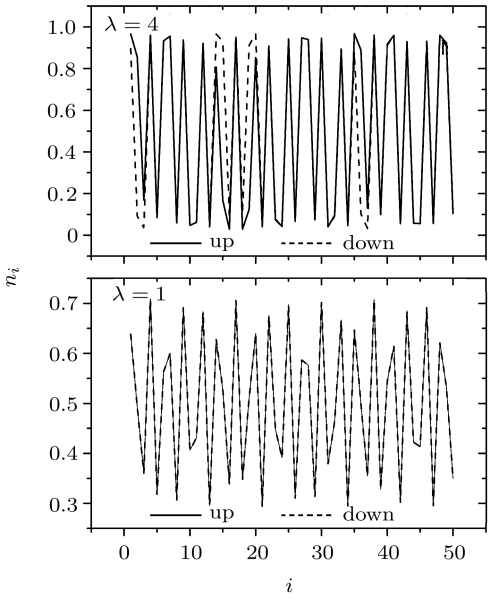



**Fig.7.** The spin densities $n_i \uparrow$ and $n_i \downarrow$, separately, versus site $i$ for a Harper Hubbard chain with values of $\lambda : 1.0$ and 4.0, $N = 50$, and $U = 1.0$.

## 5. Conclusions

In summary, we have studied one-dimensional quasiperiodic Hubbard models: Fibonacci Hubbard model and Harper Hubbard model with half filling at zero temperature by using the self-consistent Hartree-Fock approach. Because of quasiperiodicity, the usual definition of charge order parameter may not be used to describe a quasiperiodic system. So we introduce a new charge order parameter here. Then we study the properties of ground state by using a spin density wave parameter and a new charge order parameter for both models. We find that for the Fibonacci and Harper Hubbard model, there exists still a turning point $U_c$ for the CDW–SDW transition. The results show a strong competition between quasiperiodicity and electronic correlation. For a small value of $U$ (compared with the value of $\varepsilon_B - \varepsilon_A$), the CDW dominates; for a large value of $U$ (compared with the value of $\varepsilon_B - \varepsilon_A$), the SDW dominates, but the CDW does not vanish because of quasiperiodicity. While for the Harper model, when $\lambda > 2.0$ and $U < U_c$, the value of $S$ is not zero due to the localization of electronic states.

We also use the von Neumann entropy to describe ground states for both models. We find that the von Neumann entropy can be used to describe quasiperiodic models too. The turning point is indicated by the maximum value of von Neumann entropy.

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