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ELECTRONIC STATES AND PERSISTENT CURRENTS IN THE ONE-DIMENSIONAL MESOSCOPIC RINGS

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ABSTRACT

In this article the Dean's method of negative eigenvalue counting for one-dimensional chain has been extended to deal with the closed ring threaded by a magnetic flux. This new method is extremely computer memory-saving and can be used to accurately determine the eigenvalues and eigenvectors of a finite system with large number of atoms. For studying the properties of electronic states of the closed rings, we have investigated the first moment, second moment and inverse participation ratio of the wave functions for periodic, disordered and quasiperiodic systems in variety of magnetic flux and disorder degree. It is found that the second moment is an efficient parameter in the study of electronic states as well as persistent currents of the closed rings. The cluster-like structure of FM, SM, and IPR spectrum of the quasiperiodic ring as well as other interesting behaviours have been observed. The relationship between the persistent current and second moment has been studied also.

I. INTRODUCTION

The physics of small metallic rings enclosing a magnetic flux Φ is an excellent testing ground for many ideas in the field of mesoscopic physics. The energy levels, wave functions, and persistent currents have been extensively studied for many years[1-7]. Büttiker *et al.*.[2] used the transfer-matrix method to study the flux-periodic effects in one-dimensional normal-metal rings with inelastic length larger than the size of ring. Carini *et al.*[3] started from the Schrödinger equation of the mesoscopic rings by diagonalizing the Hamiltonian matrix to establish the relationship between the eigenenergy and participation ratio of the eigenvector. Cheung *et al.*[6] have also used the diagonalization method to study the persistent current I in mesoscopic rings. They have calculated I as a function of flux Φ, randomness W and temperature T. From the viewpoint of numerical simulation, a common feature in previous works is that only rather small systems were investigated, for example, the atom number of ring N=40 or less was chosen[3,6]. The primary difficulty stems directly from the fact that the diagonalization method needs huge computer memory, since the number of Hamiltonian matrix elements is N^2. Numerical diagonalizing of a large-order matrix is quite impracticable on a small computer. The total memory would require much more if the eigenenergies and

corresponding wave functions are included. This difficulty cannot be solved also by the use of the recursion method[8] or Givens-Household transformation[9], which, even though, these are very efficient technique in the field of disordered systems. One of the main purposes of this article is to present a powerful numerical approach handling very large samples of mesoscopic rings, which is based on the negative eigenvalue counting method[10] (or Dean's method) of the one-dimensional disordered chain. By the use of our approach we have successfully calculated the electronic states of a one-dimensional ring with N=2584 in a 386 personal computer. In section II we present in detail our numerical method. We will show that besides the advantage of reducing the computer memory to the same as in the original Dean's method[10,11], the improved method allows us to compute any one of the eigenvalues alone, and then calculate its corresponding eigenvector. This means that we can study some interesting eigenstates, e.g., the Fermi electronic state alone at very little cost of computer time. In section III, we report the numerical results of the isolated one-dimensional rings with ordered, disordered, and quasiperiodic lattices. We have investigated the energy eigenvalues; eigenvectors and their first moment, second moment, and inverse participation ratio (IPR), which are important parameters used to judge the localization of electronic states. It is found that the second moment is a very sensitive and efficient parameter for looking at the localization of states and describing the effects of disorder and magnetic flux on the persistent current. In the quasiperiodic lattice case, the cluster-like structure of first moment, second moment, and inverse participation ratio of wave functions are found. Other interesting results are also observed. In Section IV, we present the numerical results of the persistent currents related to the randomness W and second moment for the disordered ring threaded by magnetic flux. Section V gives a brief summary.

II. IMPROVED DEAN'S METHOD FOR THE ONE-DIMENSIONAL RINGS

For a closed ring with a magnetic fields threading the loop, (within the framework of Wannier representation) the Schrödinger equation with normalized wave function

$$|\Psi> = \sum_i a_i|i> \quad ,$$

is

$$H|\Psi> = E|\Psi> \quad , \qquad (1)$$

where

$$H = \sum_i \varepsilon_i|i> + \sum_{i,j} t_{ij}|i><j| \quad , \qquad (2)$$

The ε_i is the single-site energy and t_{ij} is the nearest-neighbor hopping integral. The matrix form of Hamiltonian is

$$H = \begin{pmatrix} \varepsilon_1 & t & & & & te^{i2\pi\frac{\phi}{\phi_0}} \\ t & \varepsilon_2 & t & & & \\ & t & \varepsilon_3 & t & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & t & \varepsilon_{n-1} & t \\ te^{-i2\pi\frac{\phi}{\phi_0}} & & & & t & \varepsilon_n \end{pmatrix} \qquad (3)$$

If the two off-diagonal elements linking the first and Nth sites equal zero, the ring reduces to an n atom chain. For solving the eigenvalue problem (1) a variety of numerical methods have been devised, the most simple one is the diagonalization method adopted extensively in previous works on the mesoscopic ring[3-7]. However, as we have mentioned, this method can only be used on small size systems if a PC computer is used, because of the memory requirements. For solving a larger system necessary to obtain a better understanding of the mesoscopic phenomena, new numerical method has to be developed. Dean's method[10] of negative eigenvalue counting has been shown to be a powerful approach, and extensively used in one-dimensional disordered single chain[11,12] and coupled chain[13]. One of the present authors (Liu) has used it to deal with the one-dimensional incommensurate systems[11] and quasilattices[14] with large number of sites.

In the rest of this section, we describe how the negative eigenvalue counting method of one-dimensional chain can be extended to tackle the one-dimensional ring problem. We will present an effective method to calculate the eigenvectors, by which the accuracy of the calculated wave function can be made to be of the same order of magnitude as that of the energy eigenvalue.

The Dean's negative eigenvalue counting method is based on a well-known theorem[15] which states that the number of negative eigenvalues of a symmetric Hermite matrix is equal to the number of changes in sign between consecutive leading principal minors, starting with the zero-order minor as positive.

For a tridiagonal matrix **M** with two off-diagonal elements linking first and Nth sites, the eigenvalue problem of the matrix **M** can be viewed as $(\mathbf{M} - x\mathbf{I})\,|\Psi\rangle = 0$

$$\boldsymbol{M} = \begin{pmatrix} a_1 & b_1 & & & & t^* \\ b_1 & a_2 & b_2 & & & \\ & b_1 & a_3 & b_3 & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & b_{n-2} & a_{n-1} & b_{n-1} \\ t & & & & & b_{n-1} & a_n \end{pmatrix}, \qquad (3)$$

where $|\Psi>$ is the eigenvector corresponding to the eigenvalue. In the Dean's method, a set of $\{u_i\}$, which are equivalent to the leading principal minors, are used to deal with the disordered chain containing large number of atoms. In the following, we present our treatment for mesoscopic ring. It shoud not be compared with the original Dean's method for straight chain.

As a first step, we decompose $\mathbf{M}$ -xI as follows

$$\mathbf{M} - x\mathbf{I} = \mathbf{L}(x)\mathbf{U}(x), \tag{4}$$

where $\mathbf{L(x)}$ is a lower triangular matrix, the elements $\mathbf{L_{ij}}$ of which are zero if i<j, and $\mathbf{U(x)}$ is an upper triangular matrix with $\mathbf{U_{ij}=0}$ if j<i. In detail, the $\mathbf{L(x)}$ and $\mathbf{U(x)}$ are chosen as follows:

$$L(x) = \begin{pmatrix} 1 & & & & & & \\ L_1 & 1 & & & & & \\ & L_2 & 1 & & & & \\ & 0 & & \ddots & & & \\ & & & & L_{n-2} & 1 & \\ y_1 & y_2 & y_3 & \cdots & y_{n-2} & L_{n-1} & 1 \end{pmatrix} \quad U(x) = \begin{pmatrix} u_1 & v_1 & & & & & z_1 \\ & u_2 & v_2 & & & & z_2 \\ & & u_3 & v_3 & & & z_3 \\ & & & \ddots & & 0 & \\ & 0 & & & u_{n-2} & v_{n-2} & z_{n-2} \\ & & & & & u_{n-1} & v_{n-1} \\ & & & & & & u_n \end{pmatrix}$$

Then, we have

$$L(x)U(x) = \begin{pmatrix} u_1 & v_1 & & & & z_1 \\ L_1u_1 & L_1v_1+u_2 & v_2 & & & L_1z_1+z_2 \\ & L_2u_2 & L_2v_2+u_3 & v_3 & 0 & L_2z_2+z_3 \\ & & \ddots & \ddots & \ddots & \\ & 0 & & L_{n-2}u_{n-2} & L_{n-2}v_{n-2}+u_{n-1} & L_{n-2}z_{n-2}+v_{n-1} \\ y_1u_1 & y_1v_1+y_2u_2 & y_2v_2+y_3 & \cdots & y_{n-2}v_{n-2}+L_{n-1}u_{n-1} & \sum_{i=1}^{n-2} y_iz_i+L_{n-1}v_{n-1}+u_n \end{pmatrix}$$

By the use of formula (4), we obtain following recursion relations used to determine the u_i v_i and L_i.

$$\left.\begin{aligned} u_1 &= a_1 - x \\ L_jv_j + u_{j+1} &= a_{j+1} - x \\ v_j &= b_j \\ L_ju_j &= b_j \end{aligned}\right\} \quad j\text{-}1, 2, 3, \ldots, n\text{-}2$$

$$\sum_{i=1}^{n-2} y_iz_i + L_{n-1}v_{n-1} + u_n = a_n - x,$$

and recursion relations used for z_i and y_i :

$$\left\{\begin{array}{l} z_1 = t^* \\ z_2 = -L_1 z_1 \\ z_3 = -L_2 z_2 \\ \vdots \\ z_{n-2} = -L_{n-3} z_{n-3} \\ L_{n-2} z_{n-2} + v_{n-1} = b_{n-1} \end{array}\right. \qquad \left\{\begin{array}{l} y_1 u_1 = t \\ y_2 u_2 = -y_1 v_1 \\ y_3 u_3 = -y_2 v_2 \\ \vdots \\ y_{n-2} u_{n-2} = -y_{n-3} v_{n-3} \\ y_{n-2} v_{n-2} + L_{n-1} u_{n-1} = b_{n-1} \end{array}\right.$$

$$\left.\begin{array}{l} z_j = -L_{j-1} z_{j-1} = \left(-\dfrac{b_{j-1}}{u_{j-1}}\right)\left(-\dfrac{b_{j-2}}{u_{j-2}}\right) \cdots \left(-\dfrac{b_1}{u_1}\right) \cdot t^* \\ y_j = -\dfrac{v_{j-1}}{u_j} y_{j-1} = \left(-\dfrac{b_{j-1}}{u_j}\right)\left(-\dfrac{b_{j-2}}{u_{j-1}}\right) \cdots \left(-\dfrac{b_1}{u_2}\right) \cdot \dfrac{t}{u_1} \end{array}\right\} \quad j = 2, 3, \ldots, n-2$$

Finally we obtain the diagonal elements of matrix **U(x)**:

$$\begin{aligned} u_1 &= a_1 - x \\ u_j &= a_j - x - \frac{b^2_{j-1}}{u_{j-1}} \qquad j = 2, 3, \ldots, n-1 \\ u_n &= a_n - x - L_{n-1} v_{n-1} - \sum_{i=1}^{n-2} y_i z_i \\ &= a_n - x - \frac{t\,t^*}{u_1} - \sum_{j=2}^{n-1} \frac{t\,t^*}{u_j} \left(\frac{b_{j-1} b_{j-2} \ldots b_1}{u_{j-1} u_{j-2} \ldots u_1}\right)^2 - \frac{b^2_{n-1}}{u_{n-1}} - (-1)^n \frac{b_{n-1} b_{n-2} \ldots b_1}{u_{n-1} u_{n-2} \ldots u_1} (t + t^*) \end{aligned} \qquad (5)$$

Because the **L(x)** is a unity mode matrix, the eigenvalue problem can be reduced to $\mathbf{U(x)}\,|\Psi\rangle = \mathbf{0}$. The negative eigenvalue theorem states that[10]

$$\eta\{M - xI\} = \sum_{i=1}^{N} \eta(u_i) .$$

Using the standard procedure of negative eigenvalue counting method, we can obtain all of the eigenvalues[10].

Now we turn process for obtaining highly accurate eigenvector. For given eigenenergy, the corresponding eigenvector is determined by the following equation:

$$\begin{pmatrix} u_1 & v_1 & & & & & \\ & u_2 & v_2 & & & 0 & \\ & & u_3 & v_3 & & & \\ & & & \ddots & \ddots & & \\ & & & & u_{n-2} & v_{n-2} & \\ & 0 & & & & u_{n-1} & v_{n-1} \\ & & & & & & u_n \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_{n-2} \\ v_{n-1} \\ u_n \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{n-2} \\ c_{n-1} \\ c_n \end{pmatrix} = 0$$

From the recursion relations(5), we can see that

$$u_j \neq 0 \quad , \qquad j = 1, 2, 3, \ldots, n\text{-}1$$

Otherwise, we can not decompose **(M-xI)** as **L(x)U(x)**. Then the **U(x)** matrix and corresponding eigenvalues would not exist. On the other hand, the existence of non-zero eigenvalue requires $\boldsymbol{det(U)=u_1u_2 \ldots u_n=0}$. Therefore, u_n must be zero for anyone of the eigenvalues. Under this condition, we can set $c_n=1$, the rest of wave function are determined by following recursion relations:

$$c_{n-1} = -\frac{v_{n-1}}{u_{n-1}} \; c_n$$

$$c_i = -\frac{v_i}{u_i} c_{i+1} - \frac{z_i}{u_i} \quad , \quad i=n\text{-}2, n\text{-}3 \ldots, 1$$

These can also be expressed in terms of the elements of **M** and **U** matrices:

$$c_{n-1} = -\frac{1}{u_{n-1}} \left[b_{n-1} + \left(-\frac{b_{n-2}}{u_{n-2}}\right) \left(-\frac{b_{n-3}}{u_{n-3}}\right) \ldots \left(-\frac{b_1}{u_1}\right) . t^* \right]$$

$$c_i = -\frac{b_i}{u_i} c_{i+1} - \frac{t^*}{u_i} \left(-\frac{b_{i-1}}{u_{i-1}}\right) \left(-\frac{b_{i-2}}{u_{i-2}}\right) \ldots \left(-\frac{b_1}{u_1}\right) \qquad (6)$$

$$i = n\text{-}2, n\text{-}3, \ldots, 1$$

After the normalizing procedure, the wave function is finally determined.

Here, we should emphasis that for the computer calculatons, the $u_n=0$ is an important criterion for obtaining an accurate wave function. We have experienced that for the finite periodic and quasiperiodic rings, the computed u_n is always close to zero for high accuracy. For the disordered rings, we can control the u_n by choosing a suitable pivoting point n. In practice, no matter how strong the disorder is, ones can easily let u_n be under 10^{-14} in order of magnitude. This method allows some very fine numerical results on the eigenvectors and related parameters to be obtained, which we will show in the next section.

III. ELECTRONIC STATES OF THE MESOSCOPIC RINGS

In this section, we report the numerical results of the one-dimensional rings enclosing a magnetic flux by the use of the improved Dean's method described in section II. We have computed three kinds of systems, i. e., periodic, disordered and quasiperiodic ones. For examining the localization of the electronic states, we have used the first moment (FM) , second moment (SM), and inverse participation ratio (IPR) to be the criterion[11,14]. Because of the geometry of the closed ring, an electron travelling the ring behaves exactly like an electron in a periodic structure, where the potential variation in one period is the same as that in one circuit around the ring. Different magnetic flux threading the ring corresponds to different boundary condition. For the mesoscopic rings, some authors have used the localization length ξ as a localization parameter[6]. Because the FM, SM and IPR are well defined and could be easily computed at the same time as the calculation of the wave function processes, we have concentrated in this paper on investigating their valuation in the adjudgment of localization.

The ith normalized eigenfunction can be expressed as

$$| \Psi_i > = \sum_{j=1}^{N} B_{ji} | \ j > \ , \tag{7}$$

Then the corresponding first moment is defined as

$$M_i = \frac{1}{N} \sum_{j=1}^{N} j B_{ji}^2 \ , \tag{8}$$

which gives the center of gravity of the wave function in the ring. We have taken the atom spacing as the unit of length. The second moment is defined as

$$S_i = \frac{1}{N} \left[\sum_{j=1}^{N} j^2 B_{ji}^2 - \left(\sum_{j=1}^{N} j \ | B_{ji} |^2 \right)^2 \right]^{\frac{1}{2}} \ , \tag{9}$$

which is a measure of the extension of the wave function. For the bound state in a one-dimensional infinite potential well, we can easily prove that the second moment equals $(12)^{-1/2} \approx 0.2886$. It has been shown that this characteristic number $12^{-1/2}$ can be also used to distinguish the extended state from the localized state and intermediate state in the one- and two-dimensional quasilattices[14,16].

The inverse participation ratio (IPR) is defined as

$$I_i = \sum_{j=1}^{N} | B_{ji} |^4 , \qquad (10)$$

which is a measure of the inverse of the number of sites occupied by the wave function. Carini *et al.*[3,4] have used the participation ratio(PR), which is the inverse of IPR, to judge the localization of electronic states of the closed rings containing site number N=3, 4, 16. In the present article the systems with N = 610 and 2584 are treated. Therefore IPR would be a more proper choice than PR, because the range of which runs from 0 to 1.

Figure 1 shows the numerical results of our improved Dean's method for periodic and disordered mesoscopic rings. The site energy ε_i is chosen to be zero for ordered rings, and randomly between -W/2 and W/2 for disordered ones. We have also taken a constant hopping matrix element t. We are considering an on-site diagonal disorder. In Fig.1 we plot the first moment, second moment, and inverse participation ratio (IPR) versus eigenenergy for a closed ring with N=610, where the thick lines represent the results of the periodic rings. For guiding the eyes, the lines have been drawn longer in the figures. Fig.1(a) shows that for the periodic ring the first moment equals 0.5, i.e., the center of gravity of wave function for all electronic states locate in the middle of the system. This means that the wave function has a homogeneous distribution in the system. If the periodic ring is changed to have a weak disorder W=0.2, we can see in the same figure that the FM spread, especially for lower and higher energy states. Fig.1(b) shows the second moment versus eigenenergy. For a periodic ring, the SM is equal to 0.2886, exactly same as that of the one-dimensional periodic chain and is represented by the thick line in the picture. Fig.1(b) shows that for a mesoscopic ring with slight disorder (W=0.2), the SM start to decrease, especially for the states located at lower and higher energy end. A smaller SM means that the electronic states becomes more localized. This trend is coincident with the general picture of the disordered systems, i.e. , the states in the middle of band are more extended. The same conclusion can be drawn from Fig.1(c), which shows the IPR versus eigenenergy. The difference is the opposite to that of the SM, the larger the IPR, the more localized the wave function.

Figure 2 shows the results of a disordered ring with randomness W=1. It shows that following the increase of degree of disorder, the FM, i.e., the center of gravity of the wave function, spread wildly in the system, the SM drop drastically, and the IPR grow up largely. This means that for such a disordered ring with W=1, the majority of the electronic states display a stronger localization so that there are only a few states. Their SM is close to 0.2886, a characteristic number of extended states. Following a further increase in the degree of disorder, the electronic states get more and more localized. Figure 3 shows the case with randomness W=2, where we can see that the FM have spread homogeneously

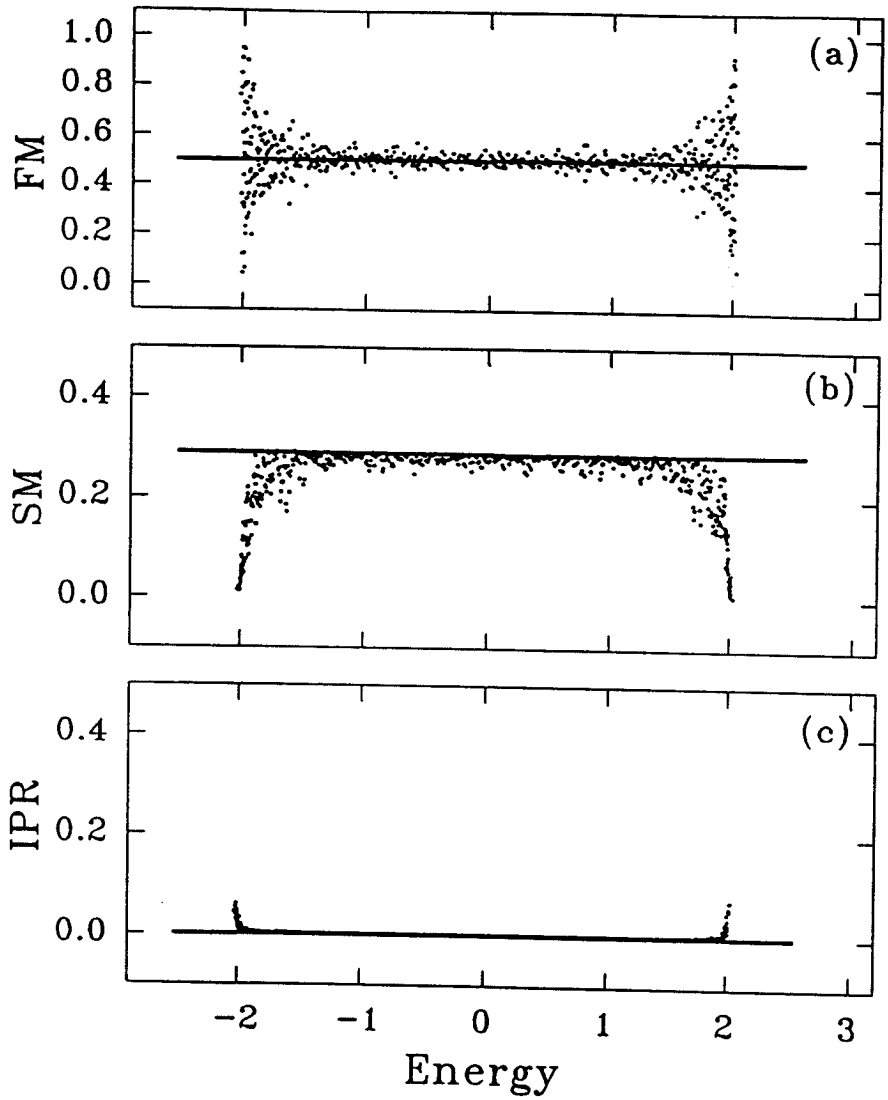

Fig.1. The first moment, second moment, and the IPR versus eigenenergy for a periodic ring (thick lines) and disordered ring (dots) with atom number N=610 and W/t=0.2 are shown, where the thick lines have been drawn longer to guide the eyes. Fig.1(a) shows that if a weak disorder is introduced the centers of gravity of the wave function will spread around 0.5, the value of periodic ring. Figure 1(b) and 1(c), which display the second moment and IPR respectively, show this kind of trend also. In the lower and higher energy ends the states spread wilder, and are more localized than those in the middle of spectrum.

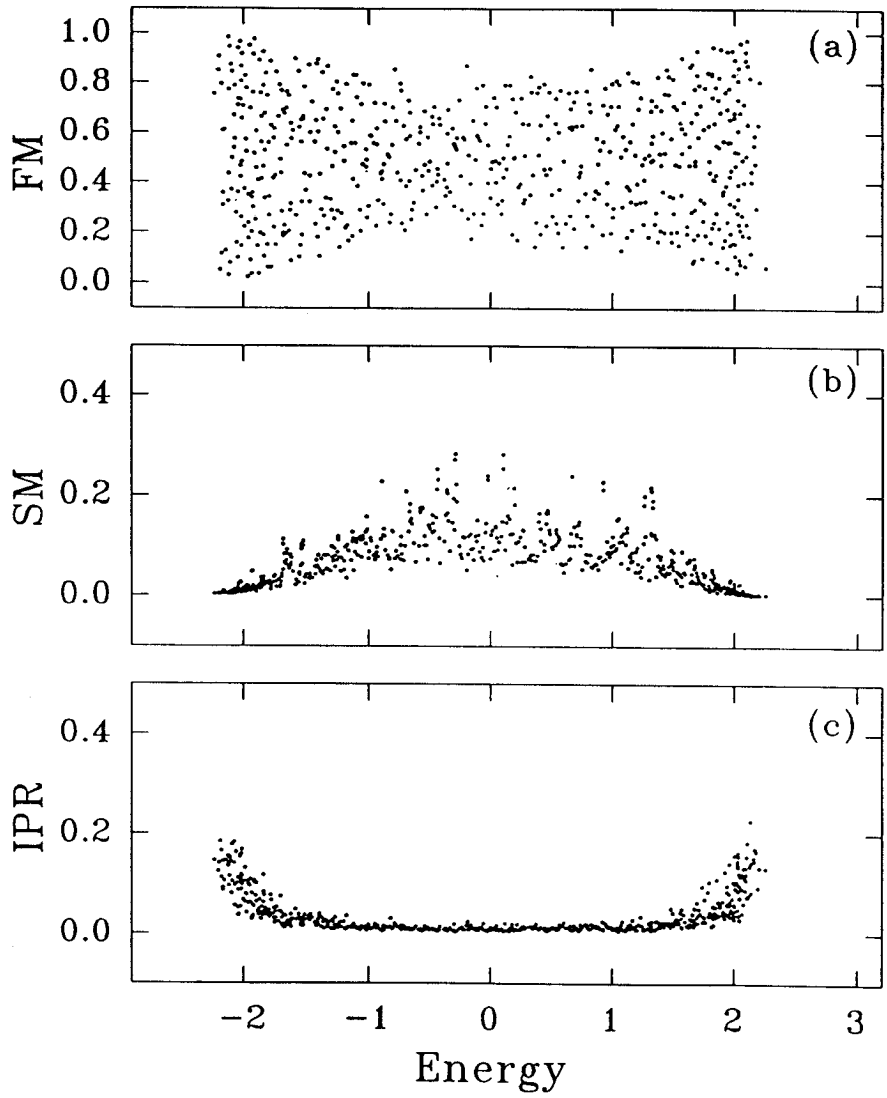

Fig.2. Same as Figure 1, but W/t=1.0 . Fig.2(a) shows that the center of gravity of the wave function spreads more homogeneously over the whole system than that of W/t=0.2 case. The electronic states in the lower and higher energy regions have changed to be localized ones. Only a few states in the middle of the spectrum their SM and IPR are still closed to 0.2886 and 1/N, respectively.

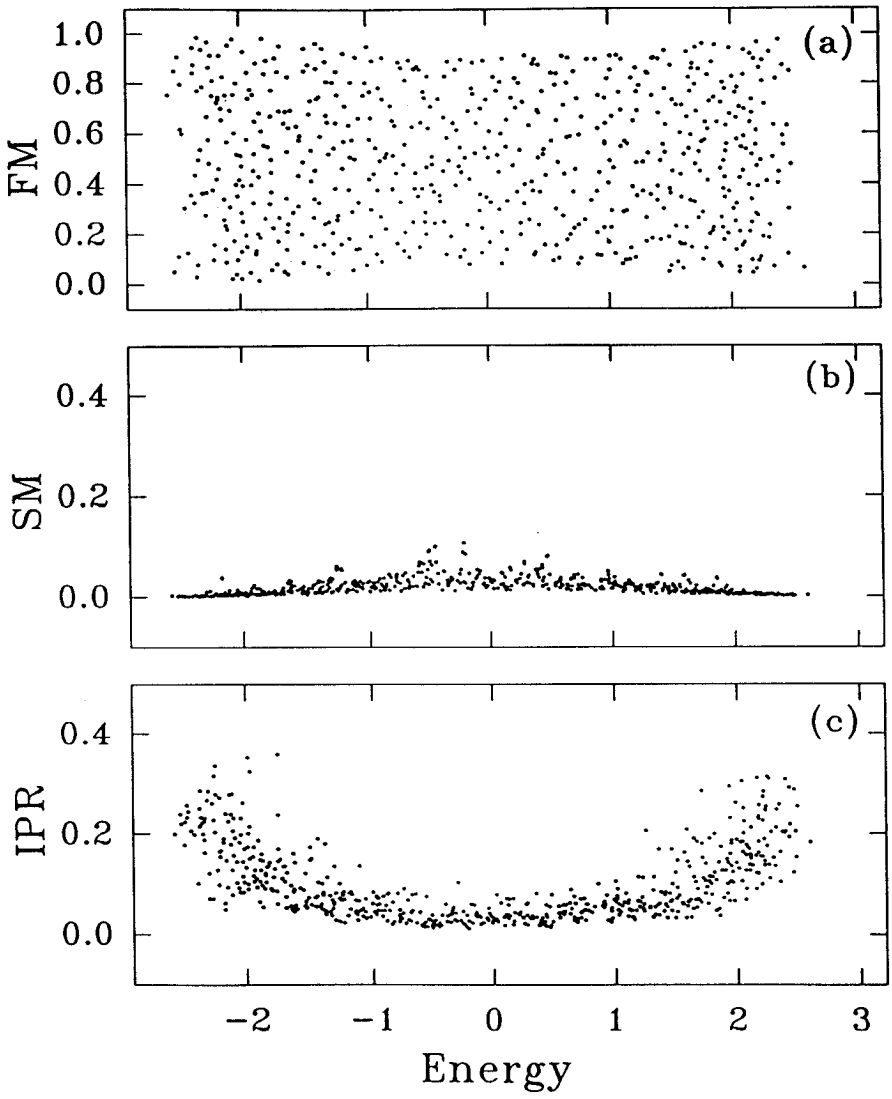

Fig.3 Same as Figure 1 and 2, but W/t=2.0. The Fig.3(a) shows that the centers of gravity of the wave functions have homogeneously spread over whole system. Fig.3(b) shows that for all of the states, the second moment is under 0.1, which implies that the states are localized. Same conclusion can be drawn also from the distribution of IPR shown in Fig.3(c).

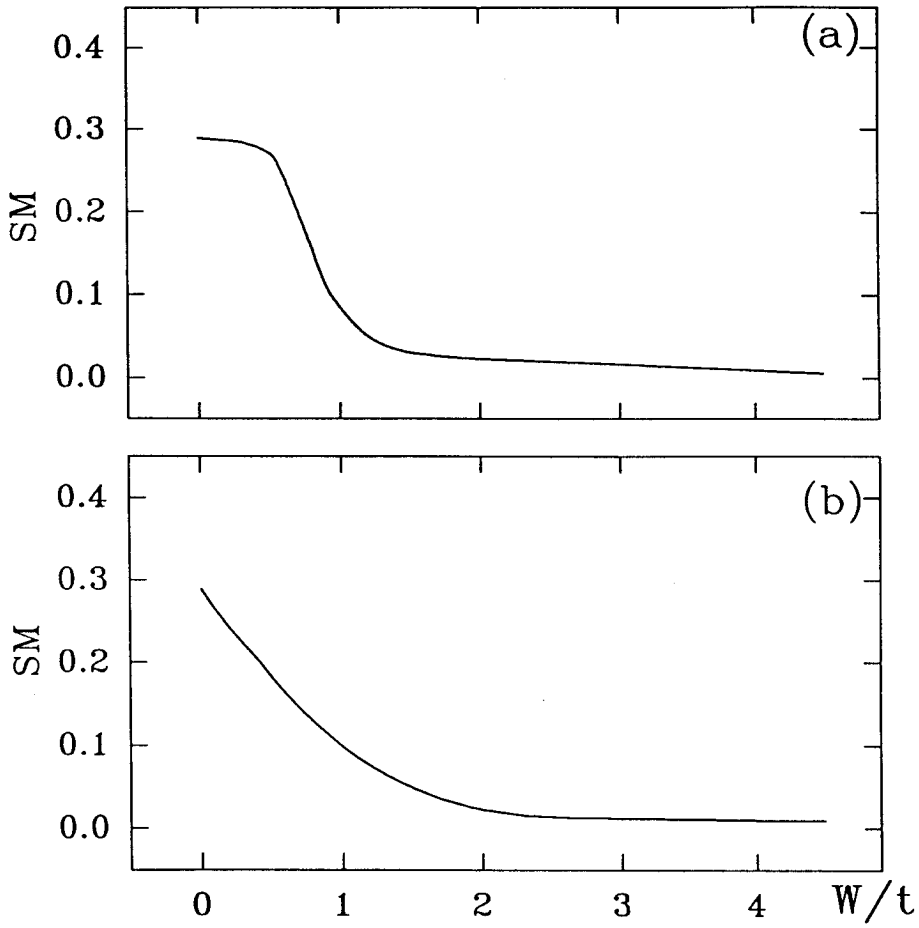

Fig.4 The second moment of Fermi electronic state versus randomness W/t for a N=610 disordered system. Fig4.(a) shows the case of closed ring threaded by flux, and (b) for the open chain. In the closed ring, the Aharonov-Bohm effect remarkably delays the decrease of SM when the disorder start to increase, then sharply drops. The crossover between weak and strong disorder appears around W/t=1.

over whole system. For all states, the SM drop to be lower than 0.1. This means that all states are localized. Showing the same trend of localization the IPR has increased drastically. We have attempted to see how this system envolves by recalculations for increasing randomness W, from 0.2 to 2 with step $\Delta W=0.1$. We found that the crossover from weak to strong localization appears roughly at $W/t=1$. This point is also supported by other calculation which be shown in the follows.

To examine further the crossover, we have computed the second moment as a function of randomness W for the Fermi electron of $N=610$ ring. The result is shown in Fig.4(a), where we can see that the SM has a big transition at $W=1$. This is in consistent with above estimation. Fig.4(b) displays the result for one-dimensional chain with same size as the ring case. Compared to the ring case, the difference is remarkable, especially in the region of W 1, i.e., the weak localization region. It means that the Aharonov-Bohm type effects postpone largely the appearance of localized state when the disorder increases.

In previous works[2-7], the relationship between persistent current and magnetic flux has been extensively studied. However, only Carini *et al.*[3] have shown numerically how the participation ratio(PR) changes following the variation of flux for $N=3,4$ and 32 small systems. Along the same line, we have investigated the relations between flux and SM, flux and IPR for longer closed ring. Figure 5 shows our numerical results of the second moment for $N=610$ disordered ring in the cases $\Phi/\Phi_0=0.25$, 0.35, and 0.45, respectively. From the figures we can see that the SM spectrum change only slightly for different Φ/Φ_0. Similar conclusion can be also drawn from the IPR spectrum. This means that the localization of electronic states does not follow the flux change.

Carini *et al.*[3] have chosen the participation ratio(PR) to study the localization of the electronic state. They found that when the ensemble average is taken, the PR does indeed have the periodicity of a half flux quantum $\Phi_0=hc/e$. Because the second moment, which is easier to be computed, is equivalent to the localization length ξ in describing the localization of wave function, it is interesting to investigate the relationship between the SM and magnetic flux for a definite electronic state. We have calculated the SM versus flux Φ/Φ_0 for the 305th eigenstate (Fermi electronic state) of the disordered mesoscopic ring with $N=610$ and $W/t=1$. The ensemble average results of SM and IPR are plotted on Fig.6. We can see that both display a perfect periodicity of a flux quantum. This is in agreement with the work by Carini *et al.*[3]. The SM curve also shows a perfect sinusoild behavior when responding to the variation of magnetic flux. The SM and IPR vibrate only in a narrow range which explains why the localization of the whole spectrum shown in Fig.5 does not change much with the variation of flux. We have also done the calculation on large system ($N=2584$), and found same behavior. It appears that this kind of fluctuation in the localization is an universal property of electronic states in the mesoscopic ring.

Following the important experiment discovery of the icosahedral symmetry in the metallic alloy Al-Mn by Shechtman *et al.*[17], the physical problems of the one-dimensional Fibonacci lattices have been extensively studied[18-20]. Many peculiar electronic properties were discovered, one of which is the self-similarity of the spectrum[14,18]. A very interesting question arises if the closed ring is formed by the Fibonacci lattice. What is the difference of its electronic properties from those of the ordered and disordered rings ?

For the transfer model of Fibonacci ring, the Hamiltonian has the same expression as (2). The site-energy is a constant, but there are two kinds of hopping integral t_A and t_B, which are arranged according to the Fibonacci sequence[14]. Fig.7 shows the numerical results of the improved Dean's method for a 15th generation Fibonacci sequence (N=610). In Fig.7(a), we plot the first moment versus eigenenergy, where we can see that the trifurcation structure is same as the finite Fibonacci chain[19,20]. At the same time, we notice that the FM, i.e., the center of gravity of wave functions, is cluster-like formed. One is around 0.38 and another around 0.72. This kind of spectral structure is very different from that of the Fibonacci **chain**, where the FM spread widely over the whole system[14], and also different from the periodic system where the FM is a straight line (see Fig.1(a)). Same cluster-like phenomenon also appears in SM and IPR spectrum shown in Fig.7(b) and (c), respectively. This kind of spectral structure could be understood if we consider that now the electrons travelling the ring see a quasiperiodic potential in a circle. The physical condition encountered by electrons is between the periodic and disordered ones. To illustrate this kind of peculiar character in Fig.8 we plot two typical wave functions, one of which has SM $\approx$ 0.72 and another one SM $\approx$ 0.38. Both of them display typical quasiperiodic fluctuation behavior[14].

IV. PERSISTENT CURRENTS

It is well-known that the current carried by level E_n at T=0 is

$$I_n = - \frac{\partial E_n}{\partial \Phi}$$

In this short section we report our numerical investigation on the relations between persistent current *I* and second moment SM as well as *I* and randomness W. Fig.9(a) shows the persistent current versus second moment for the Fermi electronic state of disordered ring with atom number N=610. To obtain the date, an ensemble average has been taken. A remarkable feature of the *I-SM* curve is that when the second moment deviates slightly from $(12)^{-1/2} \approx 0.2886$, the characteristic number corresponding to the extended states, i.e., when the system turns to be disordered from periodic one, the persistent current, undergoes immediately a very sharp drop. This point is consistent with the physical picture that the conducting current is related strongly and sensitively to the localization of the Fermi electron. The above result shows that the second moment is a very efficient parameter for the numerical study of the electronic properties of the mesoscopic rings. The second moment is very easy calculated, which the corresponding wave function is being computed. We have also investigated the effect of disorder on the persistent current. The persistent current versus the inverse of randomness W is plotted in Fig.9(b), which is in agreement with the previous work[3-7].

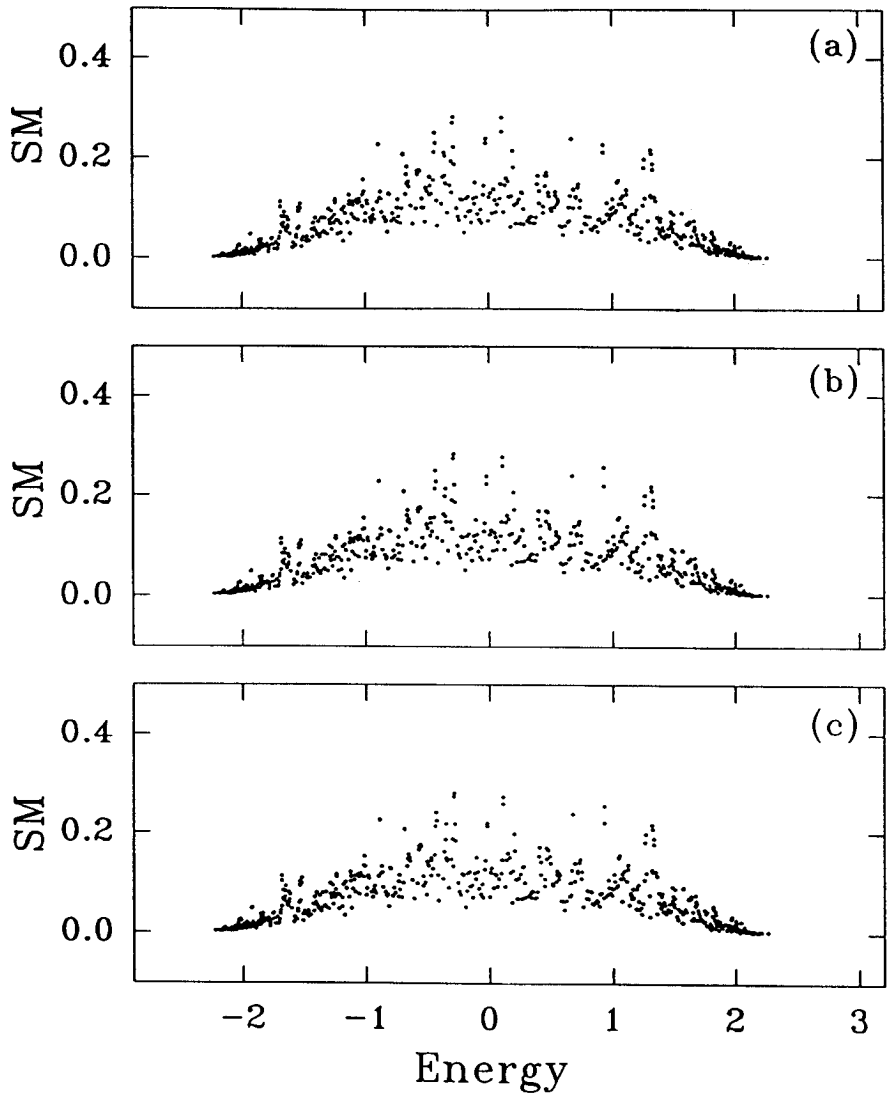

Fig.5 Same mesoscopic ring as Figure 3, W/t=1.0. In Fig.5(a),(b) ,(c), the second moment versus eigenenergy are plotted for Φ/Φ_0=0.25, 0.35 and 0.45, respectively. The pictures display that when the magnetic flux varies, the second moment spectrum changes very little. As a whole, the localization of electronic states is not sensitive to the variation of the flux.

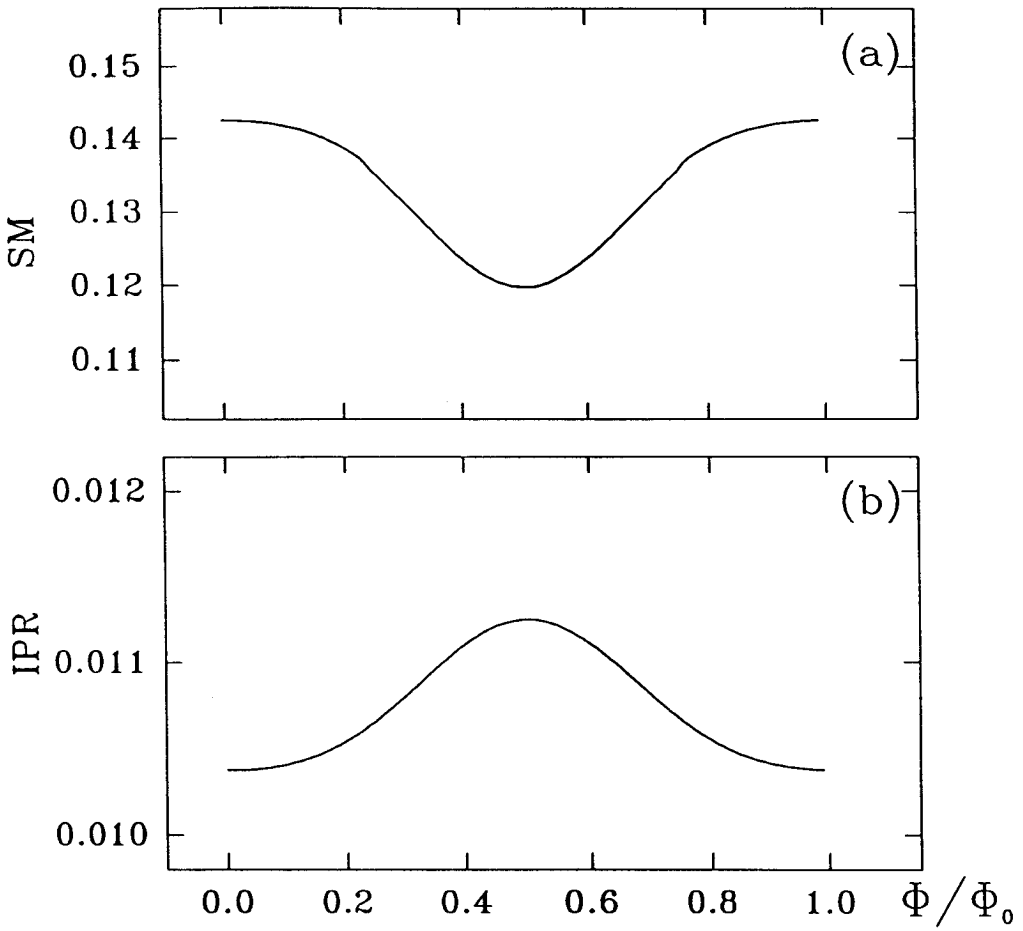

Fig.6 The second moment and inverse participation ratio of the Fermi electron for a N=610 closed ring versus magnetic flux are shown in (a) and (b), respectively. Both display the periodicity of magnetic flux quantum and perfect sinusoid behavior.

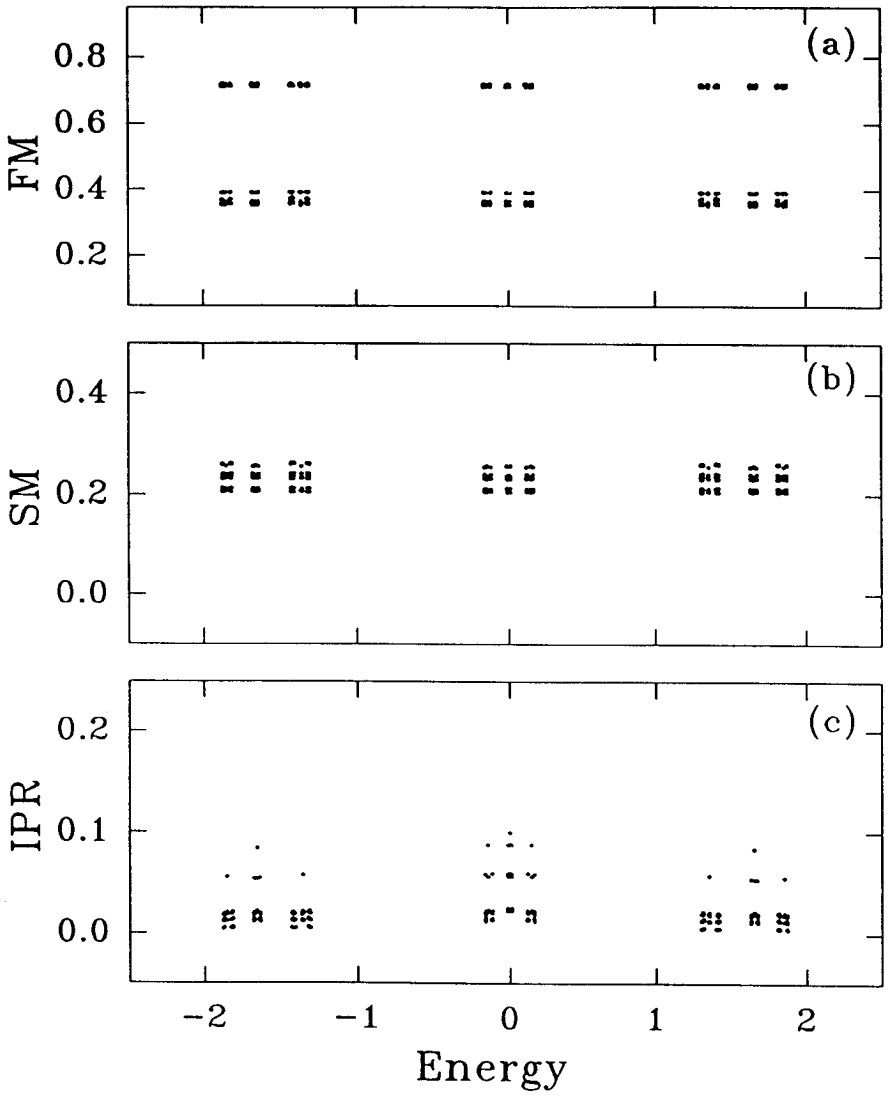

Fig.7 The first moments, second moments, and the IPR versus eigenenergy for the 15th generation Fibonacci ring with N=610 are shown, respectively. The site energy $_i$=0, the transfer matrix elements t_A=-0.5, and t_B=-1.5 have been chosen. The spectrum shows a trifurcating and cluster-like structure. (see text)

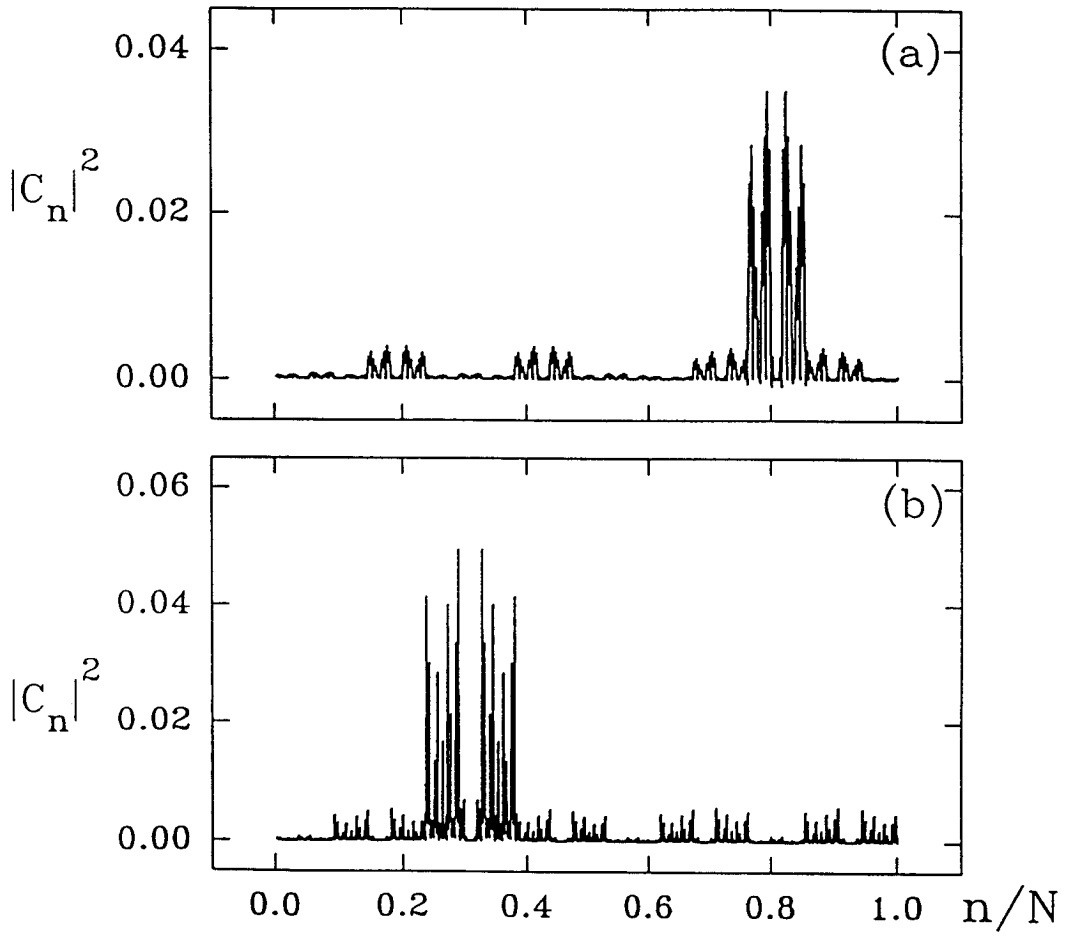

Fig.8 Two typical wave functions of same quasiperiodic system as Fig.7. The first site (n/N=0) connects with 610th site (n/N=1) to form a closed ring. Fig.8(a) shows the 202th eigenvector with E=-1.317395138425, corresponding FM 0.72. Fig. 8(b) is for the 342th eigenvector, E=0.128703318815, FM ≈ 0.38. They belong to upper and bellow cluster respectively, shown in Fig.7(a) .

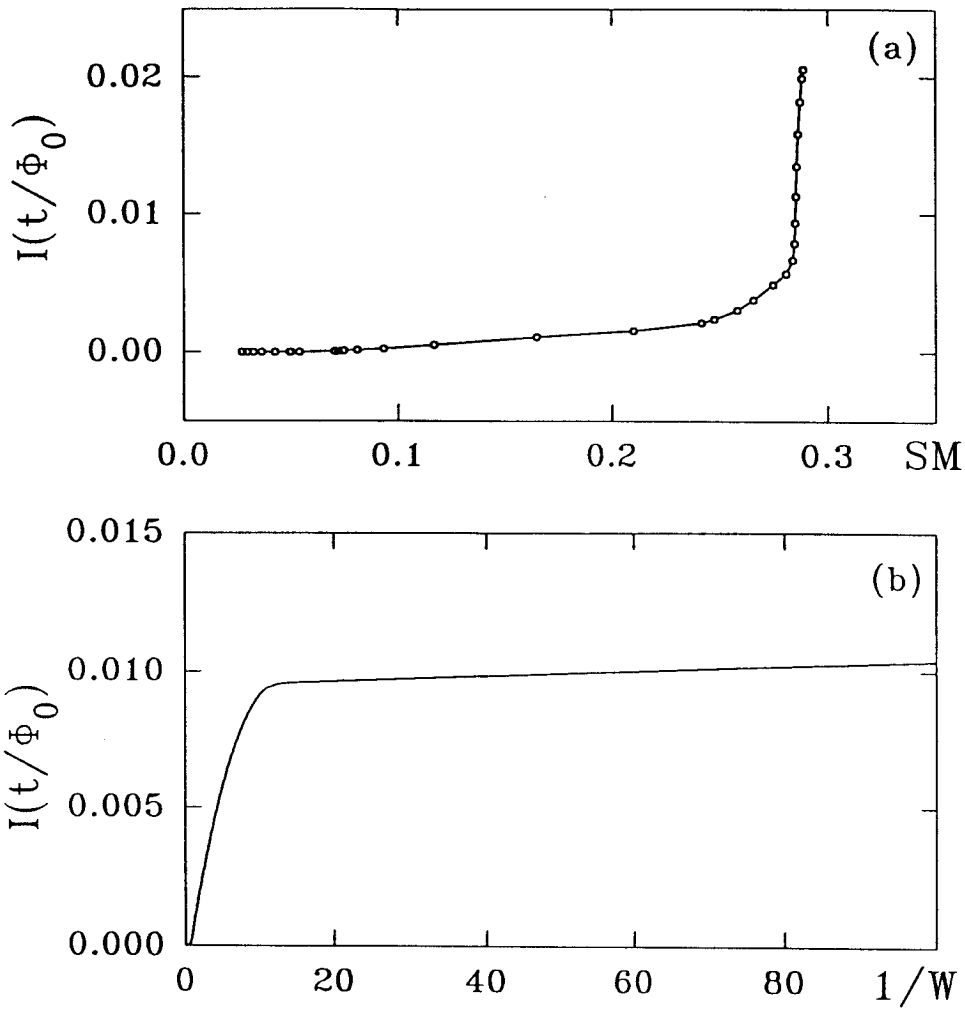

Fig.9 The persistent current versus second moment, and versus inverse of randomness for the Fermi electron of a N=610 system are shown in Fig.9(a) and (b), respectively. From (a) we can see that when the value of SM slightly leaves 0.2886, the persistent currents will very sharply drop. It represents the strong effect of the localization of electronic states on the persistent currents.

V. BRIEF SUMMARY

We have extended the Dean's method of negative eigenvalue counting for the one-dimensional disordered chain to deal with the isolated ring threaded by a magnetic flux. The improved approach allows us obtain the high accurate eigenenergies and eigenvectors for the systems with large number of atoms, which is impracticable by previous numerical approach. In this paper we have used the new method to accurately compute the eigenvalues and eigenvectors of two finite systems with N=610, and 2584 respectively, on a personal computer. Satisfactory numerical results are obtained. For investigating the localization of electronic states of the studied closed rings, the first moment, second moment, and inverse participation ratio have been computed for three kinds of systems, i. e., periodic, disordered, and quasiperiodic ones. The numerical results show that the increase of the randomness W causes the electronic states to be more and more localized. This trend is same as the case of disordered chain but the process is far slower, this being due to the Aharonov-Bohm type effect. The calculation shows a crossover from weak to strong localization at roughly a randomness value of W=1. For the quasiperiodic ring, the trifurcation structure of the energy spectrum is obtained, same as for the case of quasiperiodic chain. The cluster-like structure of FM, SM, and IPR spectrum has been found for the first time, which is very different from that of the quasiperiodic chain. The relationship between the persistent current I and SM, I and randomness W are numerically studied. The second moment shows itself to be a sensitive and efficient parameter for the numerical study of the electronic properties of the mesoscopic rings.

VI. ACKNOWLEDGMENTS

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REFERENCES

1. M. Büttiker, Y. Imry, and R. Landauer, *Phys. Lett.* **96 A**, 365 (1983).
2. M. Büttiker, Y. Imry, and M. Ya. Azbel, *Phys. Rev.* **A 30**, 1982 (1984).
3. J.P. Carini, K.A. Muttalib, and S.R. Nagel, *Phys. Rev. Lett*, **53**, 102 (1984).
4. D.A. Browner, J.P. Carini and K.A. Muttalib, *Phys. Rev.* **B 30**, 6798 (1984).
5. Q. Li and C.M. Soukoulis, *Phys. Rev.* **B 33**, 7318 (1986).
6. H.F. Cheung, Y. Gefen, E.K. Riedel, and W.H. Shih, *Phys. Rev.* **B 37**, 6050 (1988).
7. D. Kowal, V. Sivan, O. Entin-Wohlman, and Y. Imry, *Phys. Rev.* **B 42**, 9009 (1990).
8. R. Haydock, V. Heine and M.J. Kelly, *J. Phys.* **C 5**, 2845 (1972); ibid, 8, 2591 (1975).
9. R.S. Martin, C. Reinsch, J.H. Wilkinson, *Numer. Math.* **11**, 181 (1986).
10. P. Dean, Proc. Roy. Soc. A 254, 507(1960); *Rev. Mod. Phys.* **44**, 127 (1972).
11. Youyan Liu, *Phys. Rev.* **B 37**, 9694 (1988).
12. S.Y. Wu and Z.B. Zheng, *Phys. Rev.* **B 24**, 4787 (1981).
13. Z.B. Zheng, *J. Phys. C: Solid State Phys.* **20**, L 689 (1986); ibid, **20**, 4627 (1987).
14. Youyan Liu and R. Riklund, *Phys. Rev.* **B 35**, 6034 (1987).
15. H. Jefferys and B.S. Jefferys, Methods of Mathematical Physics, Cambridge U.P. Cambridge (1950).
16. Penghui Ma and Youyan Liu, *Phys. Rev.* **B 39**, 9904 (1989).
17. D.S. Shechtman, I. Blech, D. Gratias, and J.W. Chen, Phys. *Rev. Lett.* **53**, 1951 (1984).
18. M. Kohmoto, L. P. Kadanoff, and C. Tang, *Phys. Rev. Lett.* **50**, 1870 (1983).
19. Q. Niu and F. Nori, *Phys. Rev. Lett.* **57**, 2057 (1986).
20. Youyan Liu and W. Sritrakool, *Phys. Rev.* **B 43**, 1110 (1991).

บทคัดย่อ

ในบทความนี้ เราได้ขยายวิธีการของดีนที่ใช้นับค่าไอเกนลบสำหรับโซ่หนึ่งมิติให้ใช้กับวงแหวนปิดที่มีฟลักซ์แม่เหล็กพุ่งผ่านภายใน วิธีการใหม่นี้ ทำให้ประหยัดหน่วยความจำเวลาคำนวณด้วยเครื่องคอมพิวเตอร์ และยังได้ค่าไอเกนกับเวคเตอร์ไอเกนที่ถูกต้องในระบบที่มีอะตอมนับได้จำนวนมาก ในการคำนวณคุณสมบัติของสถานะของอิเล็กตรอนสำหรับวงแหวนปิดนั้น เราได้สำรวจโมเมนต์ที่หนึ่ง ที่สอง และส่วนกลับของอัตราส่วนการเข้าร่วมของฟังก์ชันคลื่นสำหรับระบบที่เป็นคาบ ที่ไร้ระเบียบ และที่เป็นเสมือนคาบ ในค่าฟลักซ์แม่เหล็กกับความไร้ระเบียบต่างๆ กัน เราได้พบว่า โมเมนต์ที่สองเป็นพารามิเตอร์ที่มีประสิทธิภาพในการศึกษาสภาวะอิเล็กตรอนเช่นเดียวกับกระแสยืนที่ในวงแหวนปิด เราได้พบโครงสร้างสเปคตรัมแบบจับกลุ่มของโมเมนต์ที่หนึ่ง ที่สอง และส่วนกลับของอัตราส่วนการเข้าร่วมของวงแหวนเสมือนคาบและคุณสมบัติที่น่าสนใจอื่นๆ นอกจากนี้ เรายังได้ศึกษาความสัมพันธ์ของกระแสคงอยู่กับโมเมนต์ที่สองด้วย