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PROCESS OF ELECTRONIC LOCALIZATION IN DISORDERED SYSTEM①

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ABSTRACT Localizability of electrons in disordered system is affected mainly by the degree of disorder and the size of system. The process of the electronic localization with the change of the two parameters was studied. There is a sharp jump for the IPR(inverse participation ratio) value which corresponds just to the formation of electronic localization. A localized state may undergo an unsteady state, which is not easy to observe, when it is changing from extended state to localized state. After a localized state is formed, the peak of the eigenvector will be split with the increase of the degree of disorder.

Key words electron localization disordered system

1 INTRODUCTION

As is well known, noninteraction electrons in disordered system are localized. Since 1958 Anderson[1] first pointed out the possibility, many researchers[2-4] investigated the topics, and a criteria of electronic localization were listed by Thouless[5]. Most works were done mainly on the properties of localized states or its scaling and conductivity.

Recently the shape and the position of localized state in disordered system were described in many papers[6-8], but the localized processes of electronic state were rarely studied, especially on the change of the localized state with disordered degree.

In order to discuss the localized process of the electronic state, the inverse participation ratio(IPR)[9] is used to describe the localized degree of electronic state in this paper. The formation of localized states was studied corresponding to the change of degree of disorder and size of system.

It is shown that an electronic state is changed from an extended state to a localized state with increase of degree of disorder. If the size of system is large enough, the states can be also localized though the degree of disorder is very weak. After a localized state is formed, its peak will split when the degree of disorder is enhanced.

2 MODEL AND METHOD

For convenience the one-dimensional Anderson disordered system will be delt with. The Hamiltonian of the Anderson model is

$$H = \sum_{i=1}^{N} \langle i | \varepsilon_i | i \rangle + \sum_{i \neq j}^{N} t_{ij} | i \rangle \langle j | \qquad (1)$$

where the basis function $| i \rangle$ is assumed to be orthonormal, N is the number of site points of the system, ε_i is a random number distributed uniformly within $(-W/2, W/2)$ and W is the degree of disorder, t_{ij} is the electronic interaction between i and j site points. Here the power law by Day and Martino[10] is applied to t_{ij}, namely:

$$t_{ij} = \begin{cases} -2/(|i-j|+1) & \text{to} \quad |i-j| \leqslant M \\ 0 & \text{to} \quad |i-j| > M \end{cases} \qquad (2)$$

M is set at 2.

For the jth eigenvalue λ_j and the eigenvector φ_j which can be expressed by the expansion of $| i \rangle$, Equation(3) can be get

$$H\varphi_j = \lambda_j \varphi_j,$$

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$$\varphi_j = \sum_{i=1}^{N} b_i | i \rangle \qquad (3)$$

From the equations 1 ~ 3, the coefficients b_i ($i = 1, 2, 3, \cdots, N$) can be calculated by

$$\begin{pmatrix} \varepsilon_1 & -1 & -2/3 & & & & \\ -1 & \varepsilon_2 & -1 & -2/3 & & & \\ -2/3 & -1 & \varepsilon_3 & \cdot & \cdot & & \\ & -2/3 & \cdot & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot & \cdot & -2/3 \\ & & & \cdot & \cdot & \cdot & -1 \\ & & & & -2/3 & -1 & \varepsilon_n \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} = \lambda_j \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} \qquad (4)$$

In order to observe the localized process of electronic state, the inverse participation ratio (IPR)[9] is introduced to express the localized degree of electronic state. The definition of IPR (R) is:

$$R = \left(\sum_{i=1}^{N} | b_i |^4\right) / \left(\sum_{i=1}^{N} | b_i |^2\right)^2 \qquad (5)$$

The $R \leqslant 1/N$ for the extended state and $1/N < R \leqslant 1$ for the localized state. Obviously the R is related to the degree of disorder W and the size of system N. The localized process of the electronic state can be known by the change of R with W and N. Here b_i are calculated by the method which can be used to solve eigenvectors of a five-diagonal matrix[11]. So the values of R can be obtained easily.

3 RESULTS AND DISCUSSION

Fig.1 shows the change of R with the degree of disorder for different size of system, which are corresponding to N = 1 000, 2000 and 5 000, respectively. The eigenvalues have been taken near to - 1. From Fig.1, it can be seen at once that (1) there is a sharp jump of IPR value in each case, which marks the beginning of electronic localization. Namely the electronic state is changing from extended state to localized state with increase of disordered degree. There are always localized states in disordered system. (2) the values of W that correspond to the jump point decrease as the size of system is increased. The jump points have moved to the left from Fig.1 (a) to (c). For example, at the jump point W is equal to 1.5 for N = 1 000 and 0.5 for N = 5 000. Both of the degree of disorder and the size of system influence each other. (3) it goes without saying, the bigger the value of R is, the stronger the degree of the electronic

Fig.1 Variation of R with degree of disorder
(eigenvalues are taken near to - 1)
(a) — N = 1 000; (b) — N = 2 000; (c) — N = 5 000

localization is. Especially when the value of R is near to 1, the electronic state is highly localized. In Fig.1(b) and (c) there are high localized states in some regions of degree of disorder. (4) the fact that the degree of electronic localization is decreased when the degree of disorder is further increased means that a split of the peak of a localized state is appeared at this time. This is also verified by the computation of eigenvectors.

It can be seen from camparing Fig.2 with Fig.1 that (1) Fig.2(a) is the same parameter as Fig.1(b), which is only enlarged at the jump area in Fig.1(b), so that the jump process is more meticulous. In the figure there is a tip of R at the jump area, which can′t be seen in Fig.1(b). It is shown that a state undergoes an unsteady state when it is being changed from a extended state to a localized state. The unsteady state is observed not easily. (2) The only difference between Fig.2(b) and Fig.1(c) is that they have different eigenvalues. In Fig.2(b) the eigenvalue is taken near to 1.7, which is at the top of the energy band, not near to -1. Compared with the two figures, the values of IPR in Fig.2(b) are larger than that in Fig.1(c). It is shown that the electronic state at the top of energy band is easier to form a localized state. In fact the states at the top and the end of energy band are produced by the degree of disorder of the system. The degree of electronic localization is very high when the eigenvalue is taken at this energy regions. In order to explain the issues above some eigenvectors of electrons in a disordered system are plotted in Fig.3.

Fig.2 Variation of R with degree of disorder
(eigenvalues X are taken near to -1 $N = 2\,000$ (a) and near to 1.7 $N = 5\,000$ (b))

Fig.3 Eigenvectors of electrons in a disordered system
(eigenvalues X are taken near to -1 (a), (b) and near to 1.7 for (c))

The parameters in Fig.3(a) and (b) are same except the degree of disorder. The peak of the localized state in Fig.3(b) has split when the degree of disorder was increased.

(2) In Fig.3(c) even though the W is equal to 0.5, the state which eigenvalue is taken near to 1.7 has been formed with high localization. It is illustrated that the results obtained are correct.

From all above, it is shown that electronic states in disordered system are localized states with the increase of the size of system. A localized state may undergo an unsteady state in the localized process with increase of the degree of disorder. After a localized state is formed, the peak of the eigenvector will be split when the degree of disorder is further increased.

REFERENCES

1 Anderson P W. Phys Rev, 1958, 109(5): 1492.
2 Abrahams E *et al*. Phys Rev Lett, 1979, 42(2): 673.
3 Mott N F. Rev Mod Phys, 1978, 50(1): 203.
4 Nagaoka Y. Prog Theor Phys, 1985, 68(Suppl 84): 1.
5 Thouless D J. J Noncryst Solids, 1972, 8 - 10(2): 461.
6 Xu Hui. Acta Phys Sinica, 1992, 41(10): 1666.
7 Xu Hui. Chin J Comput Phys, 1992, 9(3): 267.
8 Xu Hui. The Chinese Journal of Nonferrous Metals, (in Chinese), 1995, 5(Suppl 1): 84.
9 Zheng Z B. J Phys C, 1987, 20(11): 4627.
10 Day R and Martino F. J Phys C, 1981, 14(8): 4247.
11 Xu Hui. Chin J Comput Phys, 1991, 8(3): 295.

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