CHIN.PHYS.LETT. Vol.11,No.6(1994)357

# Negative Eigenvalue Counting Method for One-Dimensional Mesoscopic Rings

ZHANG Weimin, DENG Wenji, LIU Youyan
*Department of Physics, South China University of Technology, Guangzhou 510641*

(Received 16 October 1993)

*Negative eigenvalue counting method has been extended to deal with the closed ring with large number of atoms threaded by a magnetic flux. This new method is extremely computer memory-saving and can be used to accurately determine the eigenvalues and eigenvectors. As numerical examples, the results of second moment and persistent current are presented.*

*PACS: 71.25.Cx, 71.55.Jv, 72.15.Gd*

The physics of small metallic rings enclosing a magnetic flux $\Phi$ 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.[1-5] From the viewpoint of numerical simulation, a common feature in the previous work is that only rather small systems are computed, the atom number of ring $N = 40$ or even less was chosen.[2,3] The primary difficulty stems directly from that the diagonalization method needs huge computer memory, because the number of Hamiltonian matrix elements is $N^2$. To numerically diagonalize a large-order matrix is quite impractical. This difficulty can not be solved either by the use of the recursion method[6] or Givens-Household transformation,[7] which, even though, are very efficient technique in the field of disordered systems. One of the main purposes of this letter is to present a powerful numerical approach handling very large samples of mesoscopic rings, which is based on the negative eigenvalue counting method[8,9] of the one-dimensional disordered chain. Using this approach we have successfully calculated the electronic states of a one-dimensional ring with $N$=2584 on a 386 personal computer.

For a closed ring threaded by a magnetic flux, in the framework of Wannier representation the Hamiltonian is

$$H = \sum_i |i\rangle a_i \langle i| + \sum_i b_{i,i\pm1} |i\rangle\langle i \pm 1| \quad ,$$

where $a_i$ is the site energy and $b_{i,i\pm1}$ is the nearest-neighbor hopping integral. The boundary condition requires that $b_{n,1} \equiv t = c\exp(i2\pi\phi/\phi_0)$. The eigenvalue problem of the matrix $H$ can be viewed as $(H - xI)|\Psi\rangle = 0$, where $|\Psi\rangle$ is the eigenvector corresponding to the eigenvalue. As first step, we decompose $H - xI$ as

$$H - xI = L(x)\,U(x) \quad , \tag{1}$$

where

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

By Eq. (1), we obtain following recursion relations used to determine the $u_i$, $v_i$, and $L_i$:

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

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

and the recursion relations used for $z_i$ and $y_i$:

$$z_1 = t^* \ , \quad y_1 = t \cdot u_1^{-1} \ ,$$

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

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

$$\begin{aligned} u_1 &= a_1 - x \ , \\ u_j &= a_j - x - \frac{b_{j-1}^2}{u_{j-1}} \ , \quad j = 2,3,\cdots,n-1 \\ u_n &= a_n - x - L_{n-1} v_{n-1} - \sum_{i=1}^{n-2} y_i z_i \ . \end{aligned} \tag{2}$$

Because the $L(x)$ is a unity mode matrix, the studied eigenvalue problem can be reduced to $U(x)|\Psi\rangle = 0$. If $\eta\{S\}$ denotes the number of real negative eigenvalues of a matrix $S$, then the negative eigenvalue theorem states that[8]

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

Using the standard procedure of negative eigenvalue counting method, we can obtain all of the eigenvalues.[8]

For an investigated eigenenergy, the corresponding eigenvector is expressed as $(C_1, C_2, \cdots C_{n-1}, C_n)$. From the recursion relations (2), we have

$$u_j \neq 0 \ , \ j = 1, 2, 3, \cdots, n-1 \ .$$

Otherwise, we can not decompose $(M - xI)$ as $L(x)U(x)$, then the $U(x)$ matrix and corresponding eigenvalues do not exist. On the other hand, the existence of non-zero eigenvalue requires $\det(U) = u_1 u_2 \cdots u_n = 0$. 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 can be expressed by the elements of $H$ and $U$ matrices:

$$\begin{aligned} c_{n-1} &= -\frac{1}{u_{n-1}} \left[ b_{n-1} + \left( -\frac{b_{n-2}}{u_{n-2}} \right) \left( -\frac{b_{n-3}}{u_{n-3}} \right) \cdots \left( -\frac{b_1}{u_1} \right) \cdot t^* \right] \ , \\ c_i &= -\frac{b_i}{u_i} c_{i+1} - \frac{t^*}{u_i} \left( -\frac{b_{i-1}}{u_{i-1}} \right) \left( -\frac{b_{i-2}}{u_{i-2}} \right) \cdots \left( -\frac{b_1}{u_1} \right) \ , \\ & i = n-2, n-3, \cdots, 1 \ . \end{aligned} \tag{3}$$

After normalizing $c_i$, the wave function is finally determined.

We have used the above numerical method to investigate the properties of electronic states and persistent current of mesoscopic rings with $N = 610$ and 2584. As numerical examples, in this letter we only present the numerical results concerned with the second moment of wave function and persistent current. The second moment is defined as[9]

$$S_i = \frac{1}{N} \left[ \sum_{j=1}^{N} j^2 B_{ji}^2 - \left( \sum_{j=1}^{N} j |B_{ji}|^2 \right)^2 \right]^{\frac{1}{2}} \ , \tag{4}$$

which is a measure of the extension of the wave function.

For the mesoscopic rings, some authors have used the localization length $\xi$ as a localization parameter.[3] But, in fact, in the case of mesoscopic ring the localization length $\xi$ is not so well defined as the second moment of wave function. We have computed the second moment $(SM)$ as a function of randomness $W$ for the Fermi electron of $N = 610$ ring. The result is shown in Fig. 1 (a), where we can see that the $SM$ has a big transition at $W = 1$. Figure 1 (b) displays the result for the one-dimensional chain with the same size as the ring case. Comparing both of them, the difference is so remarkable especially in the region of $W \leq 1$, i.e., the weak localization region. It means that the Aharonov-Bohm effects largely postpone the appearance of localized state when the disorder increases.

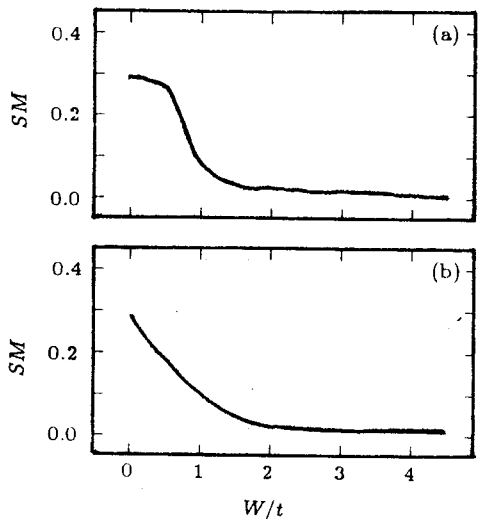


**Fig. 1.** Second moment of Fermi electronic state vs randomness $W/t$ for a $N = 610$ disordered ring. (a) For the case of closed ring threaded by magnetic flux. (b) For the open chain. In the ring case, the Aharonov-Bohm effect remarkably delays the decrease of $SM$ when the randomness increases. The crossover between weak and strong disorder appears around $W/t = 1$.

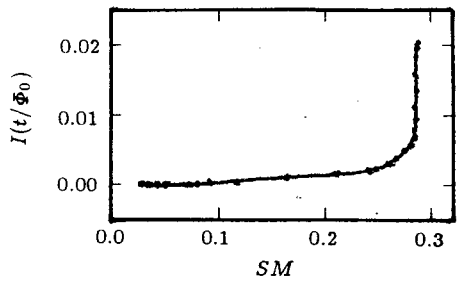


**Fig. 2.** Persistent current vs second moment for the Fermi electron of an $N = 610$ system. When the value of $SM$ slightly leaves 0.2886, the persistent currents very sharply drop. It shows the strong effect of the localization of electronic states on the persistent currents.

It is well-known that the persistent current $I_n$ carried by level $E_n$ at $T = 0$ is $I_n = -\partial E_n/\partial\phi$. Figure 2 shows the $I_n$ versus second moment for the Fermi electronic state of disordered ring with $N = 610$. To obtain the date, an ensemble average has been taken. A remarkable feature of the $I - SM$ curve is that when the second moment slightly deviates from $(12)^{-1/2} \approx 0.2886$ the characteristic number corresponding to the extended states, i. e., when the studied system turns to be disordered from periodic one, the persistent current immediately has a very sharp drop. This point coincides with the physical picture that the conducting current strongly and sensitively relates to the localization of the Fermi electron. Above two examples display that the second moment is a very efficient parameter in the numerical study of the mesoscopic rings.

## REFERENCES

[1] M.Büttiker, Y. Imry and R. Landauer, Phys. Lett. A 96 (1983) 365.
[2] J.P.Carini, K. A. Muttalib and S. R. Nagel, Phys. Rev. Lett. 53 (1984) 102.
[3] H. F. Cheung, Y. Gefen, E. K. Riedel and W. H. Shih, Phys. Rev. B 37 (1988) 6050.
[4] P. Kopietz and K. B. Efetov, Phys. Rev. B 46 (1992) 1429.
[5] M. Abraham and R. Berkovits, Phys. Rev. Lett. 70 (1993) 1509.
[6] R. Haydock, V. Heine and M. J. Kelly, J. Phys. C 5 (1972) 2845; 8 (1975) 2591.
[7] R. S. Martin, C. Reinsch and J. H. Wilkinson, Numer. Math. 11 (1986) 181.
[8] P. Dean, Proc. Roy. Soc. A 254 (1960) 507; Rev. Mod. Phys. 44 (1972) 127.
[9] Youyan Liu, Phys. Rev. B 37 (1988) 9694.