Electronic transmission properties in a mesoscopic necklace with nonlinear impurities

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(Received 2 December 1997)

The electronic transmission properties of a necklace of loop system with nonlinear impurities is studied. It shows a multivalued dependence of the transmitted intensity on the input intensity in this nonlinear system. For the transmission-energy relation, if the nonlinearity parameter is zero, there exists a range in the lower-energy region where no transmitting is permitted. If the nonlinearity parameter is nonzero, there will be transmitting peaks in the originally transmitting inhibited region of the corresponding linear system.
[S1063-651X(98)05007-7]

PACS number(s): 52.35.Mw, 73.23.−b

I. INTRODUCTION

Quantum transport through the mesoscopic systems has been extensively studied both experimentally and theoretically during the last years [1–10]. With the development of fabrication technology in semiconductors and related areas, people can fabricate devices at size smaller than the single-particle electronic coherence length. The electrons can tunnel through the samples coherently. In such mesoscopic systems, the dimension of the devices is so small that the electron transport in it is governed by quantum mechanics rather than classical mechanics and shows some interesting quantum mechanical effects, such as persistent current in isolated mesoscopic rings [5], etc. This may open a very rich field of great theoretical and experimental interest concerning these devices.

For the mesoscopic systems, the theoretical study has largely concentrated on the persistent current of isolated rings [5,6,11] and the transmission of electrons through open ring systems which are connected via leads to electron reservoirs [12–16]. In both cases, the rings are threaded by a magnetic flux Φ. In these studies, the mesoscopic systems are considered as ideal systems, and the idealized samples are treated as waveguide [14,15]. However, in reality, the ideal system is the exception rather than the rule. There may be electron-electron (e-e) interaction, electron-phonon (e-p) interaction, impurities or other defects in the real mesoscopic systems and thus the quantum mechanical effects will be affected by them. The effects of e-e interaction have been stressed by many authors and some interesting results have been obtained [11,17,18]. On the other hand, disorder in the mesoscopic systems is also considered by many authors [19,20]. But less attention was paid to the effects of e-p interaction in mesoscopic systems.

Recently, Takai and Ohta investigated the quantum oscillation and Aharonov-Bohm effect in a multiply connected normal-conductor loop [21,22] and obtained many interesting results. In their systems, rings are serially connected via a lead between two succeeding rings. In this paper we will investigate the electronic transmission properties of a mesoscopic open necklace of loop geometry [23] with nonlinear impurities. The nonlinear impurity arises from the strong local interaction between electrons and lattice vibrations in the adiabatic regime [24–27]. The necklace consists of several loops in series and each loop is threaded by a magnetic flux Φ. The nonlinear impurity is located on each loop node. The structure of it is illustrated in Fig. 1. This structure is similar to Takai and Ohta's but differs from theirs in that the succeeding rings in this model are directly connected, and our aim is to investigate the effects of nonlinearity impurities on the electronic transmission properties.

It is easy to write the equations for the wave amplitudes for the upper arm, the lower arm, and the necklace nodes as

$$E\varphi_m = e^{-i\gamma/4}\chi_{m-1} + e^{i\gamma/4}\psi_{m-1} + e^{i\gamma/4}\chi_m + e^{-i\gamma/4}\psi_m - \lambda|\varphi_m|^2\varphi_m, \tag{1}$$

$$E\chi_m = e^{-i\gamma/4}\varphi_m + e^{i\gamma/4}\varphi_{m+1}, \tag{2}$$

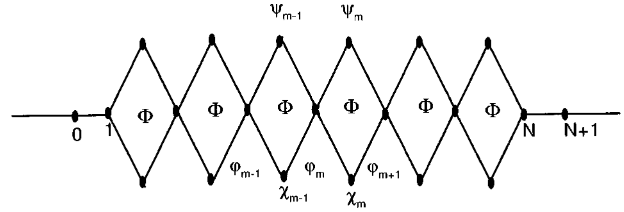

FIG. 1. The illustration of a necklace of loop geometry. It is connected to linear leads at the two ends. Each loop is threaded by magnetic flux Φ.

$$E\psi_m = e^{i\gamma/4}\varphi_m + e^{-i\gamma/4}\varphi_{m+1}, \tag{3}$$

where $\gamma = 2\pi\Phi/\Phi_0$, $\Phi_0 = h/e$, λ is the nonlinearity parameter characterizing the strength of nonlinear impurity, and E is the eigenvalue. The nearest-neighbor overlap integral is set to be 1 as a unit of energy. Eliminating χ_m and ψ_m leads to the following equation:

$$\left(E - \frac{4}{E}\right)\varphi_m - \frac{2}{E}\cos\frac{\gamma}{2}\varphi_{m-1} - \frac{2}{E}\cos\frac{\gamma}{2}\varphi_{m+1} + \lambda|\varphi_m|^2\varphi_m = 0. \tag{4}$$

II. THE NONLINEAR DYNAMICAL MAPPING

The system that will be considered here consists of a necklace of loops having N loops with nonlinear impurity on the loop nodes described by Eq. (4) embedded in an infinite one-dimensional linear periodic chain as leads. We will study the problem of stationary transmission through this nonlinear necklace. The wave function in the linear lead is taken as a single Bloch wave specified by a wave vector k. Thus

$$\varphi_m = R_0 e^{ikm} + R_1 e^{-ikm}, \quad m \leqslant 1$$

$$\left(E - \frac{4}{E}\right)\varphi_m = \frac{2}{E}\cos\frac{\gamma}{2}(\varphi_{m+1} + \varphi_{m-1}) - \lambda|\varphi_m|^2\varphi_m,$$

$$2 \leqslant m \leqslant N-1 \tag{5}$$

$$\varphi_m = Te^{ikm}, \quad m \geqslant N$$

while for the two boundaries, the equation is a little different:

$$\left(E - \frac{2}{E}\right)\varphi_N - \frac{2}{E}\cos\frac{\gamma}{2}\varphi_{N-1} - \varphi_{N+1} + \lambda|\varphi_N|^2\varphi_N = 0,$$

$$\left(E - \frac{2}{E}\right)\varphi_1 - \frac{2}{E}\cos\frac{\gamma}{2}\varphi_2 - \varphi_0 + \lambda|\varphi_1|^2\varphi_1 = 0, \tag{6}$$

where R_0, R_1, and T are defined as the incoming, reflected, and outgoing wave amplitudes, respectively. The transmission coefficient t is then given by

$$t = \frac{|T|^2}{|R_0|^2}, \tag{7}$$

and the relation $|R_0|^2 = |R_1|^2 + |T|^2$ should be required to satisfy the conservation of probability current. We can choose the overall constant phase for the wave functions so that T is real.

For this nonlinear transmission problem, it is usually not possible to define uniquely the transmission coefficient as a function of the incident intensity R_0 since there may be several combinations of (R_1, T) satisfying Eq. (5), leading to the phenomena of multistability [28,29]. To circumvent this difficulty, instead of starting from the input end, we solve the inverse transmission problem, i.e., we compute the input amplitude R_0 for the case with fixed outgoing amplitude T. We will see from Eq. (5) that R_0, R_1, and thus the transmission coefficient t can be uniquely determined by T.

Usually, φ_m should be complex variable, thus Eq. (5) gives a four-dimensional nonlinear dynamical mapping $[\mathrm{Re}(\varphi_m), \mathrm{Re}(\varphi_{m-1}), \mathrm{Im}(\varphi_m), \mathrm{Im}(\varphi_{m-1})]$. Generally, in a nonlinear dynamical mapping with degrees of freedom greater than 2, there will be a so-called Arnold diffusion [30,31]. As a result, one cannot guarantee the existence of a particular bounded orbit $(\mathrm{Re}(\varphi_m), \mathrm{Im}(\varphi_m))$ over arbitrary distance on the nonlinear system. Fortunately, thanks to the conservation of probability current $[J \equiv \mathrm{Im}(\varphi_m\varphi_{m-1}^*) = T^2 \sin k]$ in our problem, the above mapping can be reduced to a two-dimensional one, thus ruling out the possibility of the Arnold diffusion. Following Bountis *et al.* and Wan and Soukoulis [32,33], we introduce the following two variables:

$$x_m = \frac{|\varphi_m|^2}{T^2},$$

$$y_m = \frac{\mathrm{Re}(\varphi_m\varphi_{m-1}^*)}{T^2}, \tag{8}$$

and obtain the reduced nonlinear dynamical mapping for the above nonlinear system:

$$x_m = \frac{y_{m+1}^2 + (J/T^2)^2}{x_{m+1}} \quad \forall \ n,$$

$$y_m = -y_{m+1} + x_m\left(\frac{E^2-4}{2\cos\gamma/2} + \frac{E}{2\cos\gamma/2}\lambda T|^2 x_m\right), \tag{9}$$

$$2 \leqslant m \leqslant N-1.$$

At the boundaries,

$$x_N = \frac{y_{N+1}^2 + (J/T^2)^2}{x_{N+1}},$$

$$y_N = \frac{-E}{2\cos\gamma/2}y_{N+1} + x_N\left(\frac{E}{2\cos\gamma/2}\lambda|T|^2 x_N + \frac{E^2-2}{2\cos\gamma/2}\right), \tag{10}$$

$$x_1 = \frac{y_2^2 + (J/T^2)^2}{x_2},$$

$$y_1 = \frac{-E}{2\cos\gamma/2}y_2 + x_1\left[\lambda|T|^2 x_1 + \left(E - \frac{2}{E}\right)\right], \tag{11}$$

with the initial condition $x_{N+1} = 1$, $y_{N+1} = \cos k$.

From Eq. (8), we can get the expression for transmission coefficient:

$$t = \frac{4\sin^2 k}{x_1 + x_0 - 2y_1\cos k + 2\sin^2 k}, \tag{12}$$

where x_0, x_1, y_1 can be obtained by iterating Eq. (9) from the output end to the input end of the nonlinear system.

III. RESULTS AND DISCUSSIONS

The main results are shown in the figures.

In Figs. 2 and 3, we show how the input intensity varies

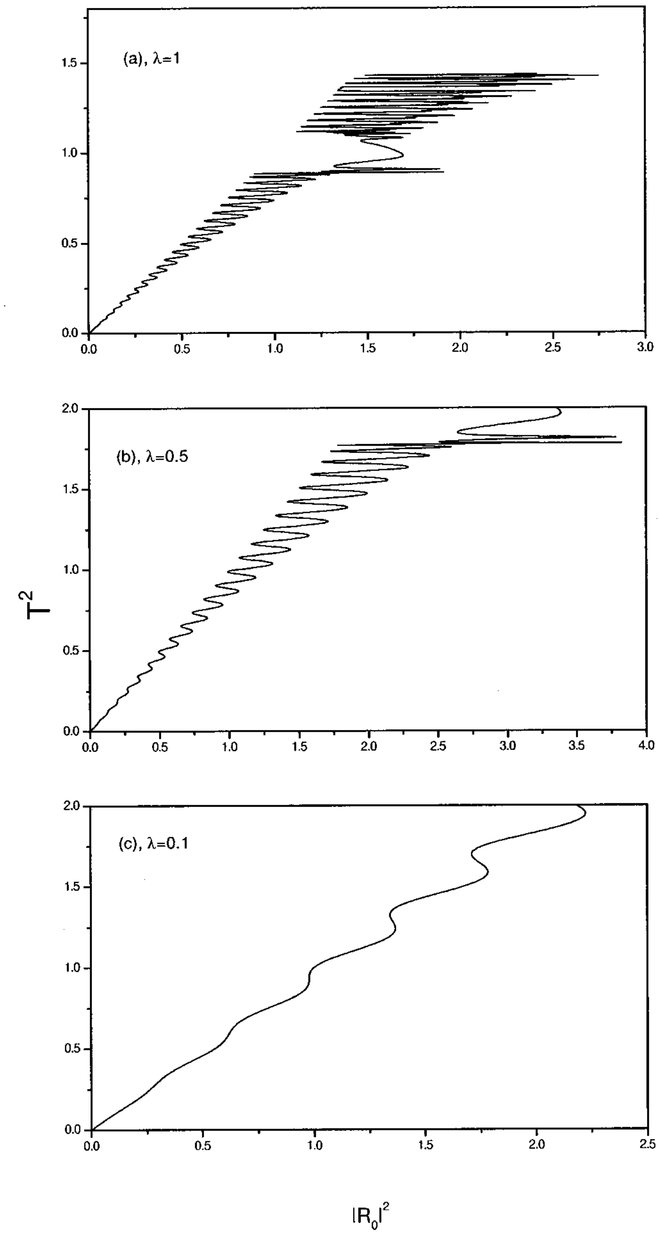

FIG. 2. The relation between T^2 and $|R_0|^2$ for different nonlinearity parameters with $\Phi=0.1\Phi_0$, and $E=1$. (a) $\lambda=1$, (b) $\lambda=0.5$, (c) $\lambda=0.1$.

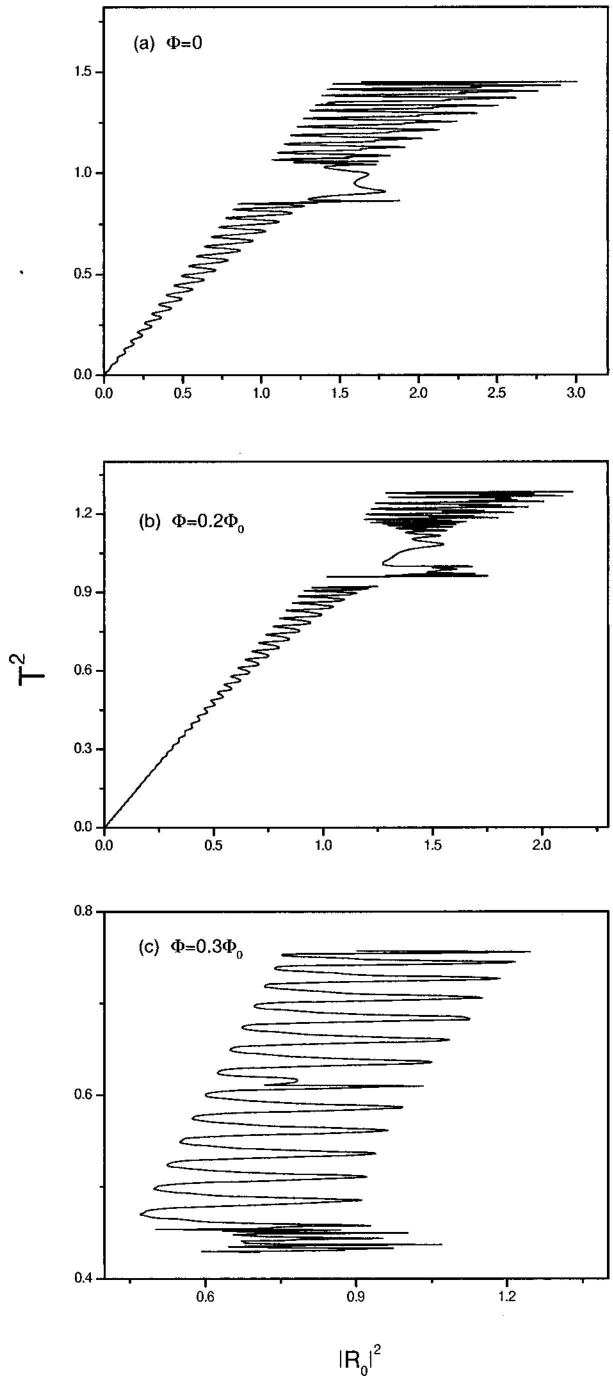

FIG. 3. The T^2–$|R_0|^2$ relation as a function of Φ with $\lambda=1$, $E=1$. (a) $\Phi=0$, (b) $\Phi=0.2\Phi_0$, (c) $\Phi=0.3\Phi_0$. Note that the transmission region in (c) is in the range $0.432\leqslant T^2\leqslant 0.757$.

with transmitted intensity with fixed energy, magnetic flux, and nonlinearity parameter.

Figure 2 is to show the effect of the magnitude of the nonlinearity parameter on the $T^2-|R_0|^2$ relation under fixed magnetic flux. We choose $E=1$, $k=\pi/3$, and magnetic flux $\Phi=0.1\Phi_0$. From the figure we can see that the incident intensity $|R_0|^2$ is a single-valued function of the transmitted intensity T^2, while T^2 is a multivalued function of $|R_0|^2$, which is the source of multistability. The multistability can result in resonant transmission, but there are interrupting smooth or monotonic regions accompanied by narrow bursts of irregular variations, especially for large T. Finally, with the increase of transmitted intensity, the incident wave amplitude diverges and thus no transmission is possible. In this case, the map entered the nontransmitting region [28].

In Fig. 3 we aim to show the effect of magnetic flux on the $T^2-|R_0|^2$ relation. In this case, $E=1.0$, $k=\pi/3$, $\lambda=1.0$. Figure 3(a) is the case with zero magnetic flux. There is no transmission gap in this figure. Figure 3(b) corresponds to a magnetic flux $\Phi=0.2\Phi_0$, we find that there is a gap in this case. For a larger magnetic flux as shown in Fig. 3(c), the gap is much larger. Now the transmitting region lies in the region $0.431\leqslant T^2\leqslant 0.758$ only. From the above results, we can see that the effect of magnetic flux on the $T-R_0$ relation is to broaden the transmission gap.

We show in Fig. 4 the transmission coefficient t as a function of energy E for given transmitted intensity T^2, magnetic flux Φ, and nonlinearity parameter λ. We see in Fig.

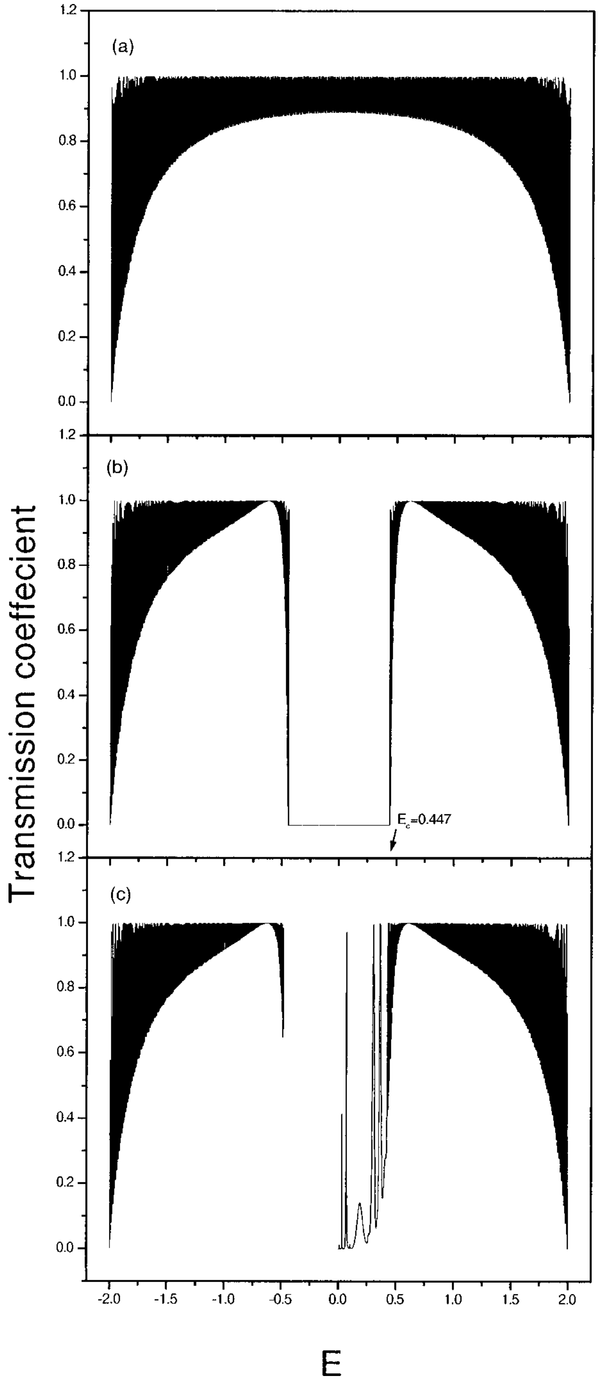

FIG. 4. Transmission coefficient t as a function of energy with fixed output intensity $T^2=0.1$. (a) $\Phi=0$, $\lambda=0$, transmission occurs when E lies between -2 and 2. (b) $\Phi=0.1\Phi_0$, $\lambda=0$, a transmission-inhibited region emerges in the range $-0.447\leqslant E\leqslant 0.447$. (c) $\Phi=0.1\Phi_0$, $\lambda=0.1$. Now transmission occurs in the positive-energy part of the inhibited region of the corresponding linear case as shown in (b).

4(a) that when no magnetic flux is added to the system and the nonlinearity parameter is 0, the transmission exists throughout the whole energy band of the linear leads $(-2.0,2.0)$ and the transmission is close to resonant transmission for the low-energy regions (deep center of the energy band). In Fig. 4(b), a magnetic flux is added but the nonlinearity parameter is 0, the transmission in the lower-energy region is inhibited, and the transmission spectral is also symmetric with respect to zero energy (the energy band center) as in Fig. 4(a). Only when the energy of the incident electron is greater than a critical value E_c does transmission occur. In this figure, $E_c=0.447$. This critical value increases with the increase of the magnetic flux until when $\Phi=0.5\Phi_0$ and transmission in the energy band of the linear leads is inhibited, then it decreases when the magnetic flux increases from $0.5\Phi_0$. As $\Phi\geqslant\Phi_0$, the above phenomenon recurs. So the critical value has a period Φ_0 in magnetic flux and it is symmetric with respect to $0.5\Phi_0$. When the nonlinearity parameter is nonzero [Fig. 4(c)], we find that there will be transmission in the inhibited region for the corresponding linear system. Moreover, transmission will occur even when the magnitude of the nonlinearity parameter is very small (for example, even when $\lambda=10^{-9}$, there still exists a transmission peak significantly greater than zero in the inhabited region for the corresponding system). In details, when λ is positive, the transmission will occur in the positive-energy region of the ''inhibited region,'' but in the negative-energy region of the ''inhibited region,'' there is no transmission phenomenon, moreover the transmission coefficient approaches zero even faster at this region than the case with zero nonlinearity parameter. In the case with negative nonlinearity parameter, this transmitting region ''moves'' to the negative-energy region of the ''inhibited region'' of the linear system, while the positive-energy region of the corresponding ''inhibited region'' is transmission inhibited. Thus the $t-E$ spectral in the case with nonzero nonlinearity parameter is no longer symmetric with respect to zero energy.

The existence of a transmission-inhibited region for the corresponding linear system can be understood by inspecting the energy band of an infinite linear necklace system threaded by a magnetic flux.

From Eq. (4), when $\lambda=0$, we can obtain the energy spectrum

$$E^2=4\left(1+\cos\frac{\gamma}{2}\cos k\right), \tag{13}$$

thus the eigenenergy of the necklace should lie in the range enclosed by the curves

$$2\sqrt{1-\cos\frac{\gamma}{2}},\quad 2\sqrt{1+\cos\frac{\gamma}{2}} \tag{14}$$

and

$$-2\sqrt{1+\cos\frac{\gamma}{2}},\quad -2\sqrt{1-\cos\frac{\gamma}{2}}, \tag{15}$$

which is plotted in Fig. 5. The permitted regions are denoted by 1,2,3,4,5,6. From the figure, we see that the permitted energy ranges from $(-2\sqrt{2},2\sqrt{2})$ when the $\Phi=0$. The energy band of the linear leads $(-2,2)$ lies in this range, so transmission can occur throughout the whole energy band of the leads. As Φ increases from 0, the permitted energy is now determined by Eq. (14) and Eq. (15), which depends on magnetic flux. If the energy of the incident electron is small, it might lie outside the permitted range, thus leading to a nontransmitting behavior. Quantitatively, as in the case in Fig. 4(b) $(\Phi=0.1)$, the critical value E_c determined from the

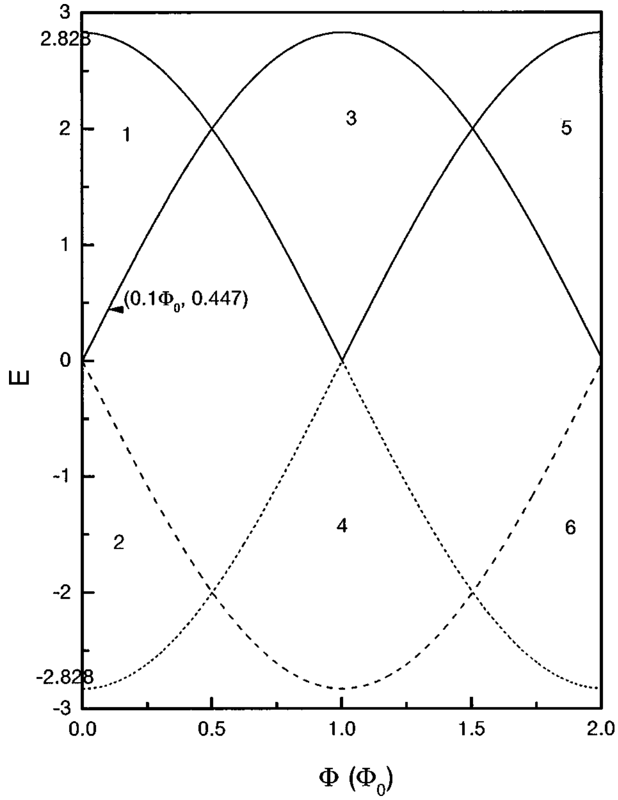

FIG. 5. The energy band of the linear infinite necklace. The permitted energy lies in the region enclosed by the curves of Eq. (14) and Eq. (15) as shown in the figure denoted by 1,2,3,4,5,6.

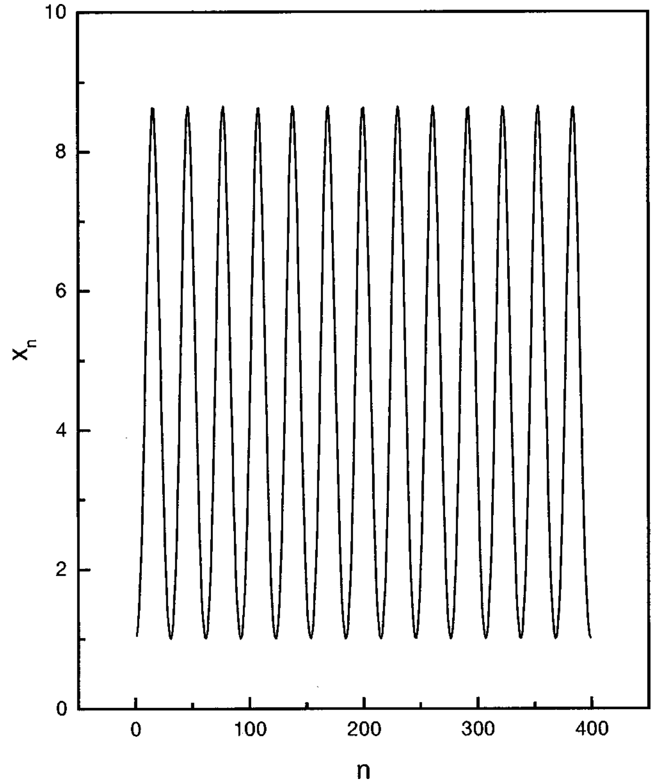

FIG. 6. The spatial distribution of electronic probability (not normalized) x_n corresponding to a transmitted behavior $t=0.997\,88$ with $E=0.4310$, $\lambda=0.1$, $T^2=0.1$, $\Phi=0.1\Phi_0$. It is an extended wave.

figure is about 0.447; from Fig. 5, the permitted range of the necklace system, we can find out that the permitted energy should be greater than or equal to 0.447, or less than or equal to -0.447. The two results are in exact agreement with each other.

The occurrence of the transmission peaks in the inhibited region for the corresponding linear system in the case with nonzero (even though it can be very small) nonlinearity parameter is the most interesting phenomenon of our result. This transmission behavior is completely due to nonlinearity and its nature is nonperturbative. It can be understood as follows. When the nonlinearity parameter is nonzero, the energy band of the necklace system has been changed. And the originally inhibited energy of the linear system may become permitted energy in the nonlinear system. Thus the electrons with energy located in the inhibited region of the linear system may tunnel through the nonlinear system inducing an excitation in it since its energy is now in the permitted region of the nonlinear system. In order to see more clearly, we show in Fig. 6 and Fig. 7 the spatial distribution of wave amplitude x_n for transmitting and nontransmitting behavior. Figure 6 corresponds to a transmitting peak at $E=0.4310,t=0.997\,88$ for $\lambda=0.1$, $\Phi=0.1$, $T^2=0.1$. We see that it is an extended wave. In Fig. 7 it corresponds to a nontransmitting behavior for the same parameters as Fig. 6 but $\lambda=0$. An important difference now appears. It is now an exponentially decaying wave function attenuating as $x_n\sim 3\times 10^{25}\exp(-n/7)$.

Figures 8 and 9 are the transmission as a function of magnetic flux for fixed energy, transmitted intensity, and nonlin-

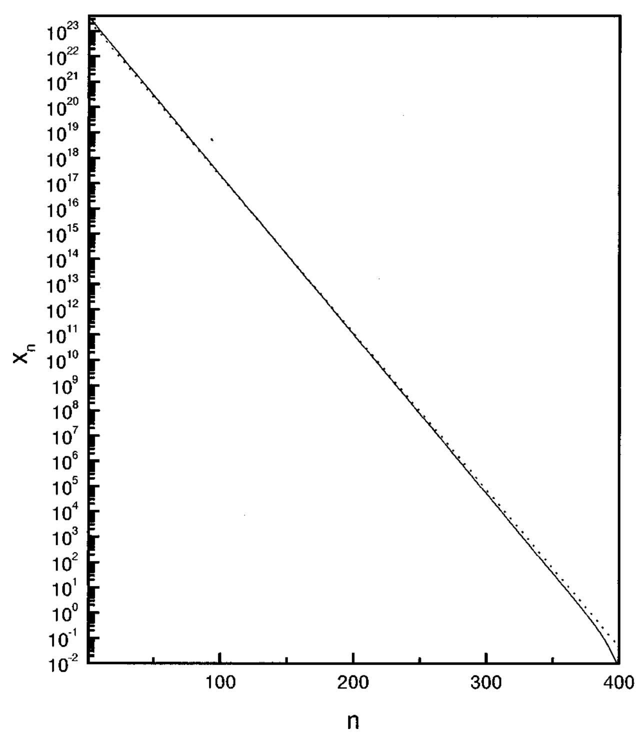

FIG. 7. The spatial distribution of electronic probability (not normalized) x_n corresponding to a nontransmitted behavior $t=0$ with $E=0.4310$, $\lambda=0$, $T^2=0.1$, $\Phi=\Phi_0$. It is an exponentially decaying wave, attenuating as $x_n\sim\exp(-n/7)$. The dotted line is the above fitting function.

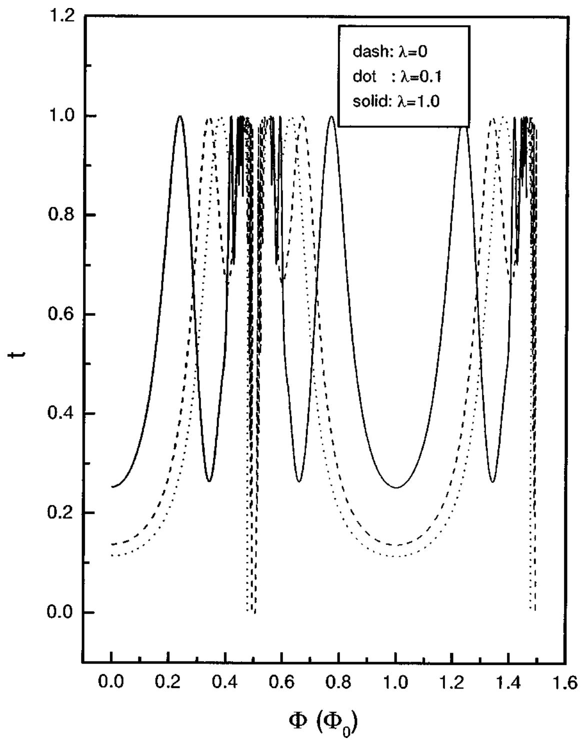

FIG. 8. The relation between t and Φ for energy near the energy band edge $E=1.98$, and $T^2=0.1$. The three curves correspond to three different nonlinearity parameters. At $\Phi=0.5\Phi_0$, they all approach zero.

earity parameter. Figure 8 is to investigate the effects of nonlinearity on the transmission spectral for the energy at the band edge of the lead with energy $E=1.98$ and fixed output intensity $T^2=0.1$. We see that the transmission coefficient is a periodic function of Φ with a period Φ_0 no matter the magnitude of the nonlinearity parameter. And we see that the transmission coefficient is symmetric with respect to $0.5\Phi_0$. When $\Phi=0.5\Phi_0$, the transmission coefficient becomes zero. In a closer look, as Φ is approaching $0.5\Phi_0$, the transmission coefficient decays to zero much more rapidly when in the case with nonzero nonlinearity parameter. This can be seen from Eq. (9). At first, we consider the case in which $\lambda=0$. When $\gamma\rightarrow\pi$, $\cos(\gamma/2)\rightarrow 0$, as a sequence, the map will diverge as $y_n\sim y_{n+1}$, thus leading to a nontransmitting behavior. When the nonlinearity parameter is nonzero, the map diverges as $y_n\sim y_{n+1}^2$, obviously, it increases much faster than the linear case for the same Φ. Physically speaking, when $\Phi=0.5\Phi_0$, the phase factor imposed by the magnetic flux on the wave function of the electrons on the two arms of a loop is π and $-\pi$, respectively, thus the outgoing wave will be suppressed due to interference. So, the transmission coefficient is extremely small. We also observe that when λ is nonzero, the position of the transmission peak is shifted from the position of transmission peak of the corresponding linear system. We also considered the case with negative λ. But numerical studies show that there is not much difference between the case with negative and positive nonlinearity parameter. It can also be seen from the previous figures that at the band edge of the lead, the transmission seems insensitive to the nonlinearity parameter since $E=2.0$ always belongs to the permitted region and the energy very close to 2.0 is

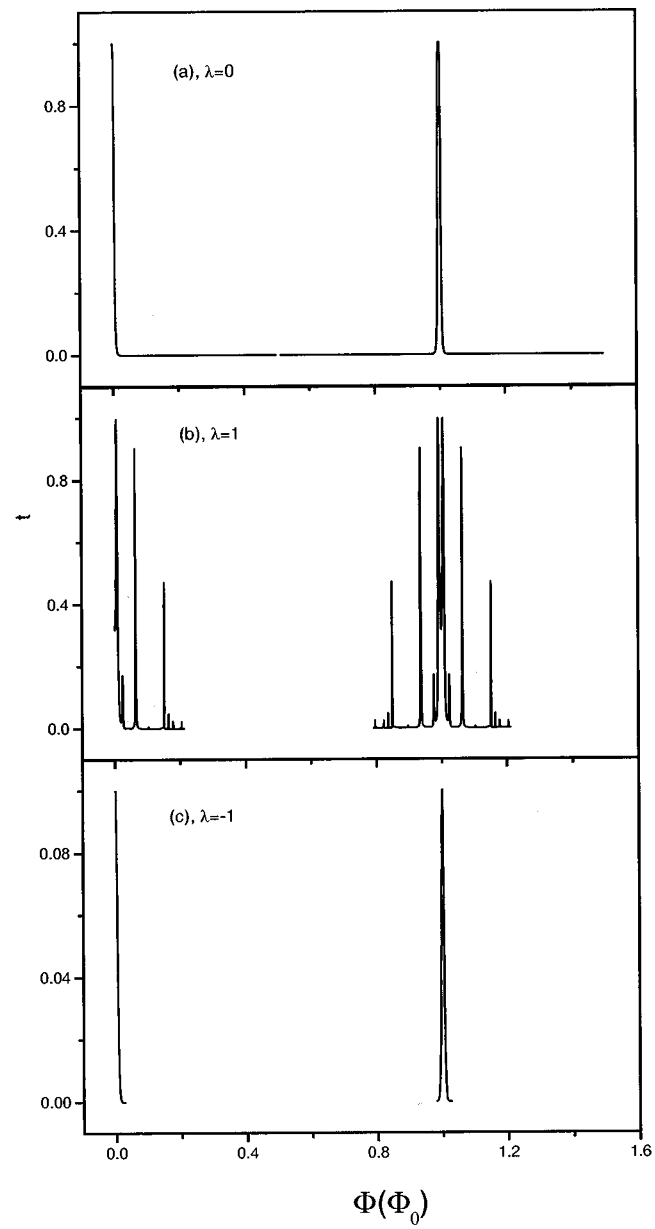

FIG. 9. The relation between t and Φ for low energy $E=0.01$. (a) $\lambda=0$, (b) $\lambda=1$, and (c) $\lambda=-1$. We can see that transmission is drastically suppressed by nonlinearity in (c).

''easy'' to be in the permitted region for any Φ (see Fig. 5).

For the case with lower energy, the results are quite different from the case at the band edge of the lead (larger energy). In Fig. 9, we plot the results of an energy $E=0.01$ and fixed output intensity $T^2=0.1$ for different nonlinearity parameters. Figure 9(a) is the case that $\lambda=0$. For this linear case, the transmission peak is very sharp, and only when Φ is very close to $k\Phi_0$ ($k=0,\pm1,\pm2,\ldots$) is the transmission coefficient significantly greater than 0. In the case of a positive nonlinearity parameter, the results are shown in Fig. 9(b). Now new peaks around the ''old'' peak emerge. The locations of these new peaks are relatively ''farther away'' from $k\Phi_0$. However, when the nonlinearity parameter is negative, which is the case of Fig. 9(c), the transmission is drastically suppressed by nonlinearity. The occurrence of transmission peak only at $k\Phi_0$ for the linear system can be understood as follows: In this case only when the magnetic flux is close to $k\Phi_0$ does $E=0.01$ belong to the permitted energy of this system; when Φ increases (or decreases) from these values, $E=0.01$ moves outside of the energy band of the necklace loop system. These results are also in agreement with that of Fig. 4, where we find that a positive nonlinearity parameter will cause ''new'' transmission peaks in the positive part of the inhibited region of the corresponding linear system and a negative nonlinearity parameter will hasten the increase of (x_n, y_n) and therefore lead to the suppression of electronic transmission in the positive part of the transmission-inhibited region. It can be implied that when $E=-0.01$, a positive nonlinearity parameter will strongly suppress the transmission while a negative one will enhance it.

In summary, we have investigated the electronic transport properties through a mesoscopic ring with nonlinear impurity at the loop nodes and obtained some interesting results. We find that the transmission behavior in this system is drastically affected by nonlinearity. In a nonlinear system, the transmission coefficient is no longer uniquely determined by input intensity but by output intensity. When the nonlinearity parameter is nonzero, there will be transmission in the transmission-inhibited region of the corresponding linear system. In detail, a positive (negative) nonlinearity will enhance the transmission of electrons with energy in the positive (negative) part of the transmission-inhibited region. These results may be useful for the fabrication of quantum devices.

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