Transport through single-channel atomic wires: Effects of connected sites on scattering phase and odd-even parity oscillations

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Theoretical studies of scattering phase and odd-even parity oscillations of the conductance are presented for a finite atomic wire system, which is either connected with two single-channel leads or side-coupled to a single-channel perfect wire. The effects of connected sites on the scattering properties are examined. For a uniform atomic wire connected with two single-channel leads, it is found that when the number of atoms in the wire, n, and the two sequence numbers of the connected atomic sites, n_1 and n_2 $(1 \leqslant n_1 \leqslant n_2 \leqslant n)$, satisfy the condition that $(n+1)/\gcd(n_1, n+1-n_2)$ is not an integer, the transmission coefficient, as a function of the incident electron energy, has zeros of second order. At these zeros the transmission phase is continuous. The zeros of the reflection coefficient, however, are always of first order, and the reflection phase has a lapse precisely by π at each of these zeros. For an atomic wire system side coupled to a perfect lead, the conclusions are reversed: the transmission zeros are always of first order, while the reflection zeros can be of high order. It is also shown that in this side-coupled configuration, both the transmission zeros and the reflection zeros are related to the generic properties of the isolated atomic wire system. The odd-even oscillations of the conductance have also been investigated for finite atomic wire systems in both configurations. It is found that the transmission of a finite atomic wire system depends not only on the parity of the number of atomic sites in the system, but also on the parity of the sequence numbers of the atomic sites through which the atomic wire system is connected with the leads. Finally, by taking a simple one-dimensional quantum wire system with several attached side branches as an example, we show that the transmission zeros of higher order can be found in a quantum system built from one-dimensional wires.

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I. INTRODUCTION

The progress in the miniaturization of electronics has stimulated numerous interest in discrete structures realized with individual atoms. A typical example among them is an atomic wire or chain, consisting of one or several atoms in a series.[1–3] The conductance through such an atomic wire sandwiched by two contacts was predicted[4–6] to show odd-even parity oscillations with the number of atoms in the wire. This feature, which has been confirmed by a recent experiment,[7] manifests the discrete characteristics of the atomic wire system. Specific odd-even parity oscillations of the conductance were also discussed for systems of a quantum dot array[8] and of a quantum ring,[9] side-coupled to a quantum wire. Very recently an atomic quantum point contact switch was demonstrated to operate at room temperature and to be entirely controlled by an external electrochemical voltage.[10] All these findings illuminate the representations of quantum effects in electron transport through atomic wire systems as well as their intriguing applications. In addition, as indicated in Ref. 11, the local probe methods allow us to build discrete systems with more complexity than atomic wires.

The odd-even parity oscillations of the conductance in atomic wire systems concern only the amplitude of transmitted electron waves. The phase properties of the electron waves are also of great importance in the characterization of the scattering problem because they contain information complementary to the scattering probability. Measurements of the transmission phase have been carried out[12,13] for a quantum channel with an attached quantum dot. It was demonstrated by Schuster *et al.*[13] that when the gate voltage applied to the dot sweeps through a conductance peak, the phase acquired by electrons traversing the quantum dot increases smoothly by π, while in the tail of a resonant peak an abrupt phase drop by π occurs. The continuous phase change by π and its profile can be well described by the Briet-Wigner resonant formula.[13] The abrupt phase drop by π was considered to be a striking phenomenon in the beginning.

Many theoretical efforts[14–23] have been made to explain the observed phase drop. Some theoretical models attempted to associate the phase drop with specific properties of the dot such as strong Coulomb repulsion,[14] asymmetric deformation,[15] and distinct difference between dot level widths.[16] In Ref. 17 a generic mechanism based on an approximate sum rule was proposed for the situation of disordered dots. The near-resonance phase lapse predicted in this model, however, is a lack of experimental evidence. Other models for the explanation of the transmission phase drop concerned the transmission zeros. It was found that the discontinuous phase change always accompanies an exact vanishing of the transmission.[18–22] It is the case even when the electron-electron interactions in the dot are taken into account.[23] In fact, this phase drop results from the generic analytical properties of the transmission coefficient around its zeros. Moreover, an important fact about the scattering phase has been clarified:[20,21] the Friedel phase, associated with the charge accumulation in the system, is not identical to the transmission phase at transmission zeros. In real systems the transmission cannot vanish exactly due to the presence of inelastic scattering. The phase drop is thus no longer sharply

discontinuous, but occurs in a narrow range of energy.[22,24] Similar discussions can be applied to the reflection phase. Numerical results in Ref. 25 indicate that both the discontinuity in the transmission phase and that in the reflection phase can occur in an atomic wire device with a cross bar configuration. Experimental studies of the transmission phase have also been made for quantum dots with Kondo correlations.[26] However, the question about a well-accepted, fundamental model for the phase property observed in the experiment by Schuster *et al.* (Ref. 13) still remains.

The vanishing of the scattering amplitude is a necessary condition for the appearance of discontinuity in the scattering phase, but not a sufficient condition.[20] It should be pointed out that the phase behavior at a scattering zero actually depends on the multiplicity of the zero. In fact, from the general formalism presented in Ref. 27, we can deduce that, as a function of the complex energy, the scattering amplitude is analytic everywhere in the complex energy plane except for at the poles of the (retarded) Green's function (GF) of the whole system. Around a real zero, E_0, the considered scattering amplitude s has a main part $s=a(E-E_0)^n$, where $a\neq 0$ and n is an integer due to the analytic property of s. When the complex energy E passes the zero E_0 in the complex energy plane[28] from the left to the right of the real energy axis, the phase will change by $-n\pi$. As a result, in the case of an odd integer n the phase difference between $s(E_0+)$ and $s(E_0-)$ is $\Delta \arg(s)=-\pi$, while for an even integer n the phase, $\arg(s)$, has no physical change at the zero E_0.

In this work we present studies of scattering properties of a single-channel atomic wire system connected by two single-channel leads and of a general atomic wire system side-coupled to a single-channel lead. We will show that for a finite atomic chain connected by two single-channel leads, all of the following three situations can happen: (1) all transmission zeros are of second order, (2) all transmission zeros are of first order, and (3) some transmission zeros are of second order, while the others are of first order. It is the integer relations among the two sequence numbers of the connected atomic sites and the number of atoms in the chain that determine which situation can occur. For a finite atomic wire system side-coupled to a single-channel lead, it will be shown that all scattering zeros are related to the generic properties of the isolated atomic wire system. The effects of the connected atomic sites on the odd-even parity oscillations of the conductance will also be examined for these atomic wire systems, and the study generalizes the results in Ref. 8. Furthermore, it will be discussed whether zeros of the order higher than 2 can be present in the transmission of a finite quantum wire system.

II. MODEL AND FORMALISM

The system under consideration is a finite atomic network (a chain, a ring, etc.) connected by two single-channel leads on the left (L) and on the right (R). In a tight-binding picture the Hamiltonian of the atomic network is given by

$$H_D=\sum_{\mathbf{r}} \varepsilon_{\mathbf{r}}|\mathbf{r}\rangle\langle\mathbf{r}| - \sum_{\mathbf{r},\mathbf{r}'} |\mathbf{r}\rangle V_{\mathbf{r},\mathbf{r}'}\langle\mathbf{r}'|, \tag{1}$$

where $\{\mathbf{r}\}$ denotes the set of the atomic sites, $\varepsilon_{\mathbf{r}}$ is the on-site energy at site $\mathbf{r}$, and $V_{\mathbf{r},\mathbf{r}'}$ is the hopping energy from $\mathbf{r}'$ to $\mathbf{r}$. The GF of the isolated system, $g(E)=(E+i\delta-H_D)^{-1}$, can be expressed in terms of the eigenstates $\{\psi_n\}$ and eigenenergies $\{E_n\}$ of the system, where $H_D\psi_n=E_n\psi_n$. In the real-space representation it is written as

$$g_{\mathbf{r}\mathbf{r}'}=\langle\mathbf{r}|g(E)|\mathbf{r}'\rangle=\lim_{\delta\to 0^+}\sum_n \frac{\psi_n(\mathbf{r})\psi_n^*(\mathbf{r}')}{E+i\delta-E_n}. \tag{2}$$

As a function of complex energy E, $g_{\mathbf{r}\mathbf{r}'}$ has poles of first order only, located at $E=E_n-i0^+$. Note that degenerate energy levels may be included in the summation of Eq. (2) when the atomic system possesses symmetries.

The atomic network couples to the left and right leads at sites A and B, respectively, via parameters v_L and v_R. The couplings are described by

$$H_C=-v_L|L\rangle\langle A|-v_R|R\rangle\langle B|+\text{H.c.}, \tag{3}$$

where $|L\rangle$ and $|R\rangle$ denote the orbital states at the surface sites of the left and right lead. The lead $\alpha(=L/R)$ is modeled as a uniform, semi-infinite, one-dimensional (1D) wire with on-site energy ε_α and nearest-neighbor interaction $t_{\boldsymbol{\alpha}}>0$,

$$H_\alpha=\sum_{n\in\boldsymbol{\alpha}}\varepsilon_\alpha|n\rangle\langle n|-\sum_{n,n+1\in\boldsymbol{\alpha}}(t_{\boldsymbol{\alpha}}|n\rangle\langle n+1|+\text{H.c.}). \tag{4}$$

The diagonal element of the GF of lead α at its surface site is given by

$$g_\alpha=(E-\epsilon_\alpha-\Sigma_\alpha)^{-1}=-t_\alpha^{-1}\exp(ik_\alpha). \tag{5}$$

Here $\Sigma_\alpha=|t_\alpha|^2 g_\alpha=-t_\alpha\exp(ik_\alpha)$ is the self-energy contribution of the remanent part in the lead to the surface site and the wave vector k_α relates with the electron energy E through $E=\epsilon_\alpha-2t_\alpha\cos k_\alpha$. An electron can propagate along the lead only when its energy falls into the window $(\epsilon_\alpha-2t_\alpha,\epsilon_\alpha+2t_\alpha)$. In the following we always assume that the electron energy E is within the region of $\cap_{\alpha=L,R}(\epsilon_\alpha-2t_\alpha,\epsilon_\alpha+2t_\alpha)$ without further specification.

For the case that electrons are incident from the left lead, the transmission coefficient $\tau=|\tau|e^{i\theta_t}$ and the reflection coefficient $r=|r|e^{i\theta_r}$ are given by[27]

$$\tau=2i\sqrt{t_R t_L\sin k_R\sin k_L}\,G_{RL}, \tag{6}$$

$$r=2it_L\sin k_L G_{LL}-1, \tag{7}$$

where G is the GF of the whole system, described by the Hamiltonian $H=H_D+H_L+H_R+H_C$, and $G_{IJ}=\langle I|G|J\rangle$. Once the transmission probability $|\tau|^2$ is known, the linear conductance $\mathcal{G}$ at zero temperature can be obtained from the one-channel Landauer-Büittker formula,

$$\mathcal{G}=|\tau|^2\mathcal{G}_0, \tag{8}$$

where $\mathcal{G}_0=2e^2/h$.

In the following we will express τ and r in terms of the matrix elements of the GF, g, through the Dyson equation. The idea is to project the GF, G, onto the subspace spanned by the states $|L\rangle$ and $|R\rangle$. The procedure employed here is the "elimination" of the center part of the system,[29] rather than the perfect leads. The effect of the center part on the electron transport is expressed in terms of the self-energy Σ_D, added

to the connected sites of the leads, of the form

$$\Sigma_D = v_L g_{AA} v_L^* |L\rangle\langle L| + v_R g_{BB} v_R^* |R\rangle\langle R| + v_L g_{AB} v_R^* |L\rangle\langle R| + v_R g_{BA} v_L^* |R\rangle\langle L|. \quad (9)$$

With the help of Σ_D and Σ_α one obtains

$$\sum_{\alpha,\beta} |\alpha\rangle G_{\alpha\beta}\langle\beta| = \left[\sum_\alpha (E - \Sigma_\alpha - \epsilon_\alpha)|\alpha\rangle\langle\alpha| - \Sigma_D\right]^{-1}. \quad (10)$$

Using the relation $E-(\epsilon_\alpha+\Sigma_\alpha)=-t_\alpha e^{-ik_\alpha}$ and after a straightforward calculation the transmission and reflection coefficients can be written as

$$\tau = 2i\sqrt{t_L t_R}\sin k_R \sin k_L \frac{g_{BA} v_R v_L^*}{\Delta}, \quad (11)$$

$$r = -\Delta^{-1}[g_{AA}|v_L|^2 t_R e^{-ik_R} + g_{BB}|v_R|^2 t_L e^{ik_L} + t_L t_R e^{i(k_L - k_R)} + \sigma|v_L v_R|^2], \quad (12)$$

where $\sigma = g_{AA}g_{BB} - |g_{BA}|^2$ and $\Delta = t_L t_R e^{-i(k_L+k_R)} + g_{AA}|v_L|^2 t_R e^{-ik_R} + g_{BB}|v_R|^2 t_L e^{-ik_L} + \sigma|v_L v_R|^2$. Along the same procedure it is possible to generalize Eqs. (11) and (12) to multichannel situations.

Equation (11) implies that a discrete transmission zero appears in two situations.[30] One is that the electron energy E coincides with a degenerate eigenenergy of the isolated system. At this energy value the denominator Δ in Eq. (11) may have a double pole so that the transmission vanishes. This kind of transmission zero is of first order. The other is that the electron energy is a zero of g_{BA}. Transmission zeros in this case can be either of first order or of high order. Note that the zeros of g_{BA} and the poles of Δ are completely determined by the isolated system and are independent of the details of the leads and the coupling parameters. Therefore, in both situations, the transmission zeros are characteristics of the isolated system, as pointed out in Ref. 22. Note that in the cross-link configuration ($A=B$) transmission zeros come only from the second situation.

One can also get the conditions for a reflection zero from Eq. (12), which is, however, cumbersome in general situations. For the symmetric coupling case of $t_L=t_R=t$, $|v_L|=|v_R|=v$, and $k_L=k_R=k$, a compact form can be obtained. In this case we have $r \propto t^2 + g_{AA}v^2 t e^{-ik} + g_{BB}v^2 t e^{ik} + \sigma v^4$. As a result, the vanishing of the reflection occurs if and only if

$$g_{AA} = g_{BB}, \quad |g_{BA}| = \left| g_{AA} + \frac{t}{v^2} e^{ik} \right|. \quad (13)$$

It can be seen from this equation that the appearance of a reflection zero, or equivalently a transmission unit, is determined by the properties of the isolated system, the leads, as well as their couplings. Thus, reflection zeros belong to the global properties of the whole structure rather than generic properties of the isolated system.

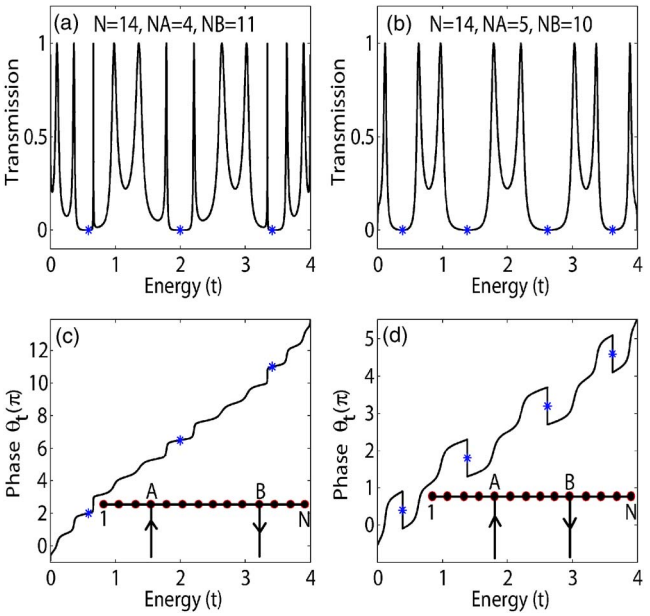

FIG. 1. (Color online) Transmission parameters (amplitude and phase) as functions of the electron energy. The considered system consists of an atomic chain of $N=14$ sites coupled to two single-channel leads at the sites n_A and $n_B=N+1-n_A$. In panels (a) and (c) $n_A=4$, while in panels (b) and (d) $n_A=5$. The points with an asterisk mark the transmission zeros. The insets in panels (c) and (d) give a schematic illustration of the corresponding devices.

III. ATOMIC CHAIN CONNECTED BY TWO SINGLE-CHANNEL LEADS

A. Scattering zeros and phase

For the two-terminal case, one of the requisite conditions for the appearance of discrete transmission zeros is the existence of two or more coherent paths[25] connecting the sites A and B. This can be visualized through the 1D chain model depicted in the insets of Figs. 1 and 2. For the 1D chain consisting of N identical atomic sites with a uniform on-site energy ε_D and hopping integral $V>0$, the eigenstates can be obtained from the boundary condition $\psi(0)=\psi(N+1)=0$. The results are

$$\psi_n(m) = \sqrt{\frac{2}{N+1}}\sin\frac{mn\pi}{N+1},$$

$$E_n = \varepsilon_D - 2V\cos\frac{n\pi}{N+1}. \quad (14)$$

The GF of the uniform 1D chain can be calculated analytically (see the Appendix). The matrix elements associated with the first and the last sites are

$$g_{11}(E) = g_{NN}(E) = \frac{\sin Nq}{-V\sin(N+1)q},$$

$$g_{1N}(E) = g_{N1}(E) = \frac{\sin q}{-V\sin(N+1)q}, \quad (15)$$

where q is given by

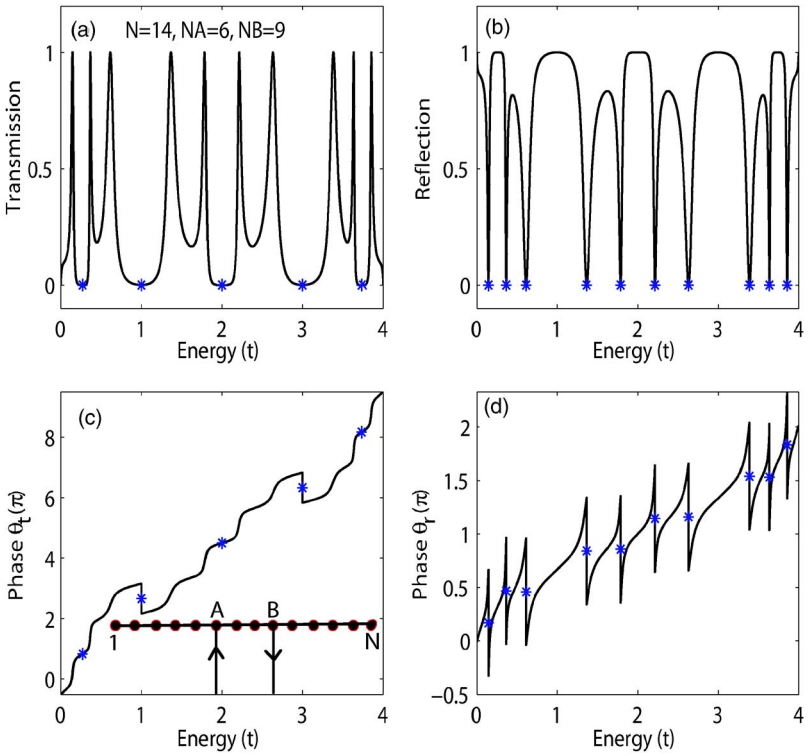

FIG. 2. (Color online) Scattering parameters (amplitude and phase of the transmission and reflection) as functions of the electron energy. The considered system consists of an atomic chain of $N=14$ sites coupled to two single-channel leads at the sites $n_A=6$ and $n_B=9$. The points with an asterisk mark the transmission or reflection zeros. The inset in panel (c) gives a schematic illustration of the corresponding device.

$$q = \cos^{-1}[(\varepsilon_D - E)/2V]. \tag{16}$$

Note again that $|\varepsilon_D - E| \leqslant 2V$. From the above equation, one can see that g_{N1} has no zero, while g_{11} has $N-1$ (first-order) zeros at $e_n = \varepsilon_D - 2V\cos(n\pi/N)$, $1 \leqslant n < N$. The reason is that for the 1D chain, g_{1N} is contributed only by the path $1 \rightarrow N$, while g_{11} is contributed by different paths. Accordingly, for the in-line configuration ($A=1$ and $B=N$) the phase of the transmission changes continuously, while for the simple cross-link (or side branch) configuration ($A=B=1$) the transmission phase has an abrupt drop by π when the electron energy passes through the value $E=e_n$.

More interesting is the case that the leads connect to one or two atoms located inside of the wire with site sequence numbers n_A and n_B ($1 \leqslant n_A \leqslant n_B \leqslant N$). In Fig. 1 both the amplitude and the phase of the transmission are plotted as a function of the electron energy for a chain of $N=14$ atomic sites connected by two single-channel leads through site n_A and site $n_B = N+1-n_A$. Two values of n_A are considered: $n_A=4$ in panels (a) and (c) and $n_A=5$ in panels (b) and (d). The parameters are chosen as $t_L=t_R=V=t$, $v_L=v_R=0.5t$, and $\varepsilon_D=\varepsilon_L=\varepsilon_R=2t$. From the transmission spectrum we can see that both the number of resonant peaks and the number of zeros depend on the connected sites. It is known that for the in-line configuration ($n_A=1$), there are 14 transmission resonances and no transmission zeros.[25] Here it is seen that for $n_A=4$ there are 12 resonant peaks and 3 zeros, while for $n_A=5$ there are 8 resonant peaks and 4 zeros. The phase shift of the transmission coefficient for $n_A=4$ shows a rather different variation with the electron energy E, in comparison with that for $n_A=5$ [see Figs. 1(c) and 1(d)]. In the case of $n_A=5$, the transmission phase drops by π precisely when the transmission coefficient passes through each of its zeros. This observation is in agreement with previous studies. As for the case of $n_A=4$, however, the phase changes continuously with the electron energy E, even in the presence of transmission zeros. This indicates that a zero of the transmission does not necessarily lead to a lapse of the transmission phase.

Can both the continuity and discontinuity of the transmission phase at the transmission zeros be observed in the same device? The answer is shown in Fig. 2, where the amplitude and phase of the transmission and reflection are plotted for the same structure as in Fig. 1, but with different connected sites, $n_A=6$ and $n_B=9$. From panel (c) one can see that the transmission phase has a drop by π at some transmission zeros, while at the other zeros it changes continuously. As a comparison the reflection phase is presented in panel (d) for the same structure. One can see that at each reflection zero the phase of the reflection coefficient has a drop by π. This observation agrees with the results in Ref. 25.

The numerical calculations presented above can be understood analytically as follows. For the situation that the sequence numbers of the connected sites satisfy the condition $n_A+n_B=N+1$ (which we call "symmetric link"), the element g_{BA} is

$$g_{BA} = \frac{\sin^2(n_A q)}{-V\sin[(N+1)q]\sin q}. \tag{17}$$

Thus g_{BA} has zeros at $\varepsilon_p = \varepsilon_D - 2V\cos(p\pi/n_A)$, with the integer p satisfying $1 \leqslant p < n_A$. These zeros can be either of first order or of second order: the zero of g_{BA} at ε_p is of second order when $p(N+1)/n_A \notin Z$ and is of first order otherwise. According to this rule three situations can be identified for the variation of the transmission phase with the electron energy. The integer relation between $N+1$ and n_A determines

which situation will occur. For the situation $\gcd(N+1,n_A)=1$ all the zeros of g_{BA} are of second order. The transmission phase thus changes continuously at all of these zeros, as is seen in Figs. 1(a) and 1(c). For the situation $(N+1)/n_A \in Z$ all the zeros of g_{BA} are of first order. The transmission phase thus has a drop by π at each of these zeros, as is seen in Figs. 1(b) and 1(d). For the situation $1<\gcd(N+1,n_A)<n_A$ some of the zeros of g_{BA} are of first order while the other zeros are of second order. The transmission phase thus has a drop by π at some of these zeros and changes continuously at the other zeros, as is seen in Figs. 2(a) and 2(c). These facts manifest the complication of the destructive interference even for a simple 1D chain. For the situation $n_A+n_B \neq N+1$, the location and multiplicity of transmission zeros depend on three integers, n_A, n_B, and N. From Eq. (A6) one can prove that for the case of $(N+1)/\gcd(n_A,N+1-n_B) \notin Z$, there exists at least one transmission zero of second order. As for the reflection coefficient, since its zeros come from the poles of the GF of the whole system, they are always of first order. As a result, the reflection phase has a drop by π at each of these zeros, as is seen in Figs. 2(b) and 2(d).

B. Odd-even oscillations of the conductance

We discuss the odd-even oscillations only for the case of symmetric coupling ($v_L=v_R=v$, $t_L=t_R=t$, and $k_L=k_R=k$) and symmetric links ($n_A+n_B=N+1$), and consider the transmission (or, equivalently, reflection) variation with the number of atomic sites in the atomic chain, N, and the sequence number of the coupling site, n_A, at the fixed electron energy $E=\varepsilon_D$. Equation (13) may be applied to determine whether the reflection vanishes at $E=\varepsilon_D$. For the case of symmetric links one always has $g_{AA}=g_{BB}$, which is the first condition in Eq. (13). Whether or not the second condition in Eq. (13) is satisfied depends on the parity of N and n_A. For an even N, the second condition in Eq. (13) at $E=\varepsilon_D$ becomes $\sin^2(n_A\pi/2)=tV/v^2$, which can be satisfied only when the coupling strength v is exactly $(tV)^{1/2}$. When this is the case and n_A is odd, the reflection is zero and the transmission is the unit. However, in the situations studied in Figs. 1 and 2, $v=t/2=V/2$ and thus $v \neq (tV)^{1/2}$. The transmission at $E=\varepsilon_D(=2t)$ should not approach the unit as is seen in Figs. 1 and 2. For an odd N and an even n_A, g_{BA} and g_{AA} vanish at $E=\varepsilon_D$. In this situation the second condition in Eq. (13) is again not satisfied and thus the transmission cannot approach the unit. For the situation that both N and n_A are odd, Eq. (13) cannot be applied to determine whether or not the reflection vanishes at the energy $E=\varepsilon_D$, because both g_{BA} and g_{AA} have a pole at this energy. However, in this case, $\sigma=g_{AA}g_{BB}-|g_{BA}|^2$ is bounded, i.e., $\lim_{E\to\varepsilon_D}|\sigma(E)|<\infty$, and Eq. (12) can be simplified as

$$r=-e^{2ik}\frac{(t+\sigma v^4/t)g_{AA}^{-1}+2v^2\cos k}{(t+\sigma v^4/t)g_{AA}^{-1}+2v^2e^{ik}}=-e^{ik}\cos k. \quad (18)$$

When the atomic chain and the two leads have the same on-site energy ($\varepsilon_D=\varepsilon_L=\varepsilon_R$), one has $k=\pi/2$ at $E=\varepsilon_D$. Under this condition Eq. (18) implies that the reflection is always zero and the transmission is always one, independent of the coupling strength. Also, in this situation the phase of the reflection coefficient always has a drop by π at $E=\varepsilon_D$.

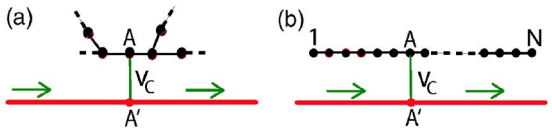

FIG. 3. (Color online) Schematic illustration of side-coupled atomic systems: (a) general situation and (b) an atomic wire with a finite atomic number N.

The above parity-dependent transmission and reflection phenomena can clearly be viewed as a kind of odd-even oscillation.[4–6] Here the occurrence of odd-even oscillations requires that at least one of the two conditions, $v=(tV)^{1/2}$ and $\varepsilon_D=\varepsilon_L=\varepsilon_R$, should be satisfied. The rules of the parity oscillations under different situations can be summarized as follows. For the situation that both conditions mentioned above are satisfied, the odd-even oscillations depend only on the integer n_A,

$$\mathcal{G}(E=\varepsilon_D)\begin{cases}=\mathcal{G}_0, & \text{odd } n_A,\\ <\mathcal{G}_0, & \text{even } n_A.\end{cases} \quad (19)$$

Under the other two situations the parity oscillations are determined by both n_A and N. If only the condition $v=(tV)^{1/2}$ is satisfied, one has

$$\mathcal{G}(E=\varepsilon_D)\begin{cases}=\mathcal{G}_0, & \text{odd } n_A \text{ and even } N,\\ <\mathcal{G}_0, & \text{otherwise}.\end{cases} \quad (20)$$

However, if only the condition $\varepsilon_D=\varepsilon_L=\varepsilon_R$ is satisfied, one has

$$\mathcal{G}(E=\varepsilon_D)\begin{cases}=\mathcal{G}_0, & \text{odd } n_A \text{ and odd } N,\\ <\mathcal{G}_0, & \text{otherwise}.\end{cases} \quad (21)$$

IV. ATOMIC SYSTEM SIDE-COUPLED TO A SINGLE-CHANNEL PERFECT WIRE

A. Scattering zeros and phase

In this subsection, we discuss the scattering problem for the structure of a general finite atomic wire system side-coupled to a perfect single-channel atomic wire as sketched in Fig. 3(a). In Sec. IV B we apply the results of this subsection to a simple case in which the finite atomic wire system is simply a 1D atomic chain. In the perfect wire the on-site energy is ε_0 and the hopping integral is t. The finite atomic system and the perfect wire are coupled through site A in the atomic system and site A' in the wire with the coupling strength v_C. To proceed, we add the site A' to the original finite atomic wire system to get a larger one. Thus, Eqs. (11) and (12) hold if the replacement, $g_{AA}\to(E-\varepsilon_0-|v_C|^2g_{AA})^{-1}$, and the parameter settings, $t_L=t_R=v_L=v_R=t$ and $k_L=k_R=k(\epsilon_L=\epsilon_R=\epsilon_0)$, are made. The simplified results are

$$\tau=e^{2ik}\frac{2it\sin k}{2it\sin k-|v_C|^2g_{AA}}, \quad (22)$$

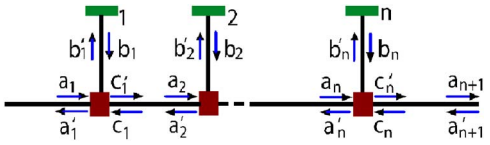

FIG. 4. (Color online) Current amplitudes for the model of a wire attached by n identical side branches of length L_B with an equal distance L_W between adjacent junctions.

$$r = e^{2ik}\frac{|v_C|^2 g_{AA}}{2it\sin k - |v_C|^2 g_{AA}}. \tag{23}$$

From these two equations we have the following conclusions for the coherent electron transport through a side-coupled system.

(1) In contrast to the in-line or crossbar configuration, here all (discrete) transmission zeros occur at eigenenergies E_n of the isolated system (the poles of g_{AA}). Note, however, that the transmission is truly zero at $E=E_n$ only if the local density of states at the atomic site A, $\rho_A(E_n)=\Sigma_m \delta(E_m - E_n)|\psi_m(A)|^2$ with $\{\psi_m\}$ being the eigenfunctions of the isolated atomic system, is nonvanishing. Some special examples of this conclusion have been reported.[8,9]

(2) The vanishing of the reflection occurs at zero of g_{AA} [Eq. (23)].

(3) All the transmission zeros are of first order, the transmission phase thus has a drop by π at each of them. Therefore, measurements of the phase acquired by transmitted electrons can give the energy level structure of the isolated system. The reflection zeros, however, may be of high order due to the complicated destructive interference. It should be noted that for this side-coupled atomic system both the transmission zeros and the reflection zeros are related to generic properties of the isolated system.

(4) The wave function information of the eigenstates can be detected through conductance measurements in the neighborhood of the transmission zeros. In fact, at energy E around a nondegenerate energy level E_n, the conductance has the form

$$\mathcal{G}(E) = \frac{(E-E_n)^2[4t^2 - (\varepsilon_0 - E_n)^2]}{|v_C|^4|\psi_n(A)|^4}\mathcal{G}_0, \tag{24}$$

if the eigenfunction ψ_n is nonvanishing at the coupling site A.

B. Side-coupled 1D chain

As an example, we reconsider a 1D atomic chain model, which is now side-coupled to a perfect wire through the atom located at site n_A [see Fig. 3(b)]. In this case the diagonal element of the GF, g_{AA}, is of interest and is given by

$$g_{AA} = \frac{\sin(n_A q)\sin[(N+1-n_A)q]}{-V\sin[(N+1)q]\sin q}. \tag{25}$$

The transmission resonances and antiresonances can be easily determined from Eqs. (22) and (23). There are $N - \gcd(n_A, N+1)$ resonances at $q=n\pi/n_A$ $(1\leqslant n<n_A)$ or $q=m\pi/(N+1-n_A)$ $(1\leqslant m<N+1-n_A)$, and $N+1-\gcd(n_A,N+1)$ antiresonances at $q=n\pi/(N+1)$ $[1\leqslant n\leqslant N, n\times\gcd(n_A, N+1)/(N+1)\notin Z]$. As a result, when the electron energy is fixed at the value of $E=\varepsilon_D$, the odd-even parity oscillations of the conductance can occur, but in a different fashion:

$$\mathcal{G}(E=\varepsilon_D) = \begin{cases} 0, & \text{odd } n_A \text{ and odd } N, \\ \mathcal{G}_0, & \text{otherwise}. \end{cases} \tag{26}$$

Accordingly, the reflection phase always changes by π at $E=\varepsilon_D$ when either of n_A and N is even. The special $n_A=1$ case has been discussed in Ref. 8. Note that here both the transmission zeros and the reflection zeros are of first order.

V. HIGH-ORDER TRANSMISSION ZEROS

So far, we have shown that the transmission of a finite atomic wire system can have zeros of first order, second order, or both. The question whether higher-order transmission zeros can occur in a finite quantum wire system is certainly of interest to study. Here we intend to provide an intuitive answer to the question by considering a simple, well-studied, 1D system with several identical side branches,[18–20,31] as depicted in Fig. 4. We will show that it is possible to observe zeros of high order (higher than 2) in the transmission through a finite quantum wire system.

For a 1D lead attached by n identical side branches of length L_B with an equal distance L_W between adjacent junctions (Fig. 4), the wave amplitudes (a'_1, a_{n+1}) are related with (a_1, a'_{n+1}) by a 2×2 scattering matrix S_n, whose off-diagonal elements give the transmission coefficient τ_n. The scattering problem for a 1D wire attached by a single side branch has been studied and the scattering matrix S_1 of the single side-branch system has been derived.[18–20,32] From Ref. 18 we know that τ_1 has zeros of the first order at the wave vector $k_m=m\pi/L_B$, $m=1,2,3,\ldots$. These transmission zeros are Fano-type antiresonances, which are due to the interaction between the discrete levels in the side branch and a continuous band from the straight 1D channel.

For $n>1$, the composition law[33] of the scattering matrix gives $\tau_n=\tau_1^n/f_n$, where f_n can be a function of the transmission coefficient τ_1, the reflection coefficient r_1, as well as L_W. The transmission thus may have zeros of an arbitrary order at $\{k_m\}$. Here the actual multiplicity of transmission zeros is determined by a single real parameter, L_W/L_B. Note that if and only if $\exp(2m\pi i L_W/L_B)=1$, the zero at k_m has an order lower than n. In this situation the zero is actually of first order. As a result, for an irrational L_W/L_B, all zeros at $\{k_m\}$ have the order of n. For an integer value of L_W/L_B, all zeros at $\{k_m\}$ are of first order. For the case that L_W/L_B is rational but not integer, some of the zeros have the order of n, while the others are of first order.

The atomic chain systems considered in Sec. III can be viewed as a special kind of side-branch system (see the insets in Figs. 1 and 2). The part located on the left side of site A and the part located on the right side of site B in each studied atomic chain model in Sec. III can be considered as two attached branches. Since there are only two side branches, the highest order of transmission zeros in this model is 2, as can be seen from Eqs. (11) and (A6).

VI. CONCLUSIONS

In summary, we have studied scattering phase properties and odd-even parity oscillations of the conductance of finite atomic wire systems with different configurations of the connections to the perfect leads. For a finite atomic chain attached with two single-channel leads we have shown that the transmission has zeros of second order and its phase does not have a drop at these zeros. In contrast, the zeros of the reflection of the system are always of first order and the reflection phase shows a lapse of π at each of the reflection zeros. It has also been shown that the transmission zeros are characteristics of the generic property of the isolated atomic wire system, while the reflection zeros are related to the global properties of the whole structure rather than the isolated system alone. For an atomic wire system side coupled to a single-channel lead, the conclusions for scattering zeros are reversed: The transmission zeros are always of first order, while the reflection zeros can be of higher order. Also in this side-coupled configuration both the transmission zeros and the reflection zeros are related to the generic properties of the isolated atomic wire system. The odd-even oscillations of the conductance have also been investigated for finite atomic wire systems in both configurations. It is found that the transmission of a finite atomic chain depends not only on the parity of the number of atomic sites in the chain, but also on the parity of the sequence numbers of the atomic sites through which the atomic chain is connected with the leads. Finally we have shown the existence of higher-order zeros in the transmission through a 1D wire system with several identical side branches attached. It is shown that at certain given electron energies the transmission of the system can have zeros of the order identical to the number of side branches in the system and, therefore, the phase drop at these zeros is determined by the parity of this number.

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APPENDIX: GREEN'S FUNCTION OF A FINITE 1D CHAIN

In this appendix we briefly show how to obtain the GF of a uniform atomic chain with a finite length. This can be done by using the following lemma twice.

Lemma. If a system described by the Hamiltonian H can be divided into two subsystems described by the Hamiltonians, H_0 and H_1, so that interaction exists only between their surface sites 0 and 1, the GF, $G^0=(E-H_0)^{-1}$, can be expressed in terms of the GF, $G=(E-H)^{-1}$, through

$$G^0_{mn} = G_{mn} - G_{m1}G^{-1}_{11}G_{1n}, \tag{A1}$$

where m and n are site indices in the subsystem 0.

The lemma can be easily proved. By writing $H=H_0+H_1+V_{01}|0\rangle\langle 1|+V_{10}|1\rangle\langle 0|$, one can obtain the following relations from the Dyson equation:

$$G_{mn} = G^0_{mn} + G^0_{m0}V_{01}G_{1n}, \quad G_{m1} = G^0_{m0}V_{01}G_{11}, \tag{A2}$$

which immediately give Eq. (A1).

The uniform chain with a finite length N is described by the Hamiltonian

$$H_{1N} = \sum_{1\leqslant n\leqslant N} \varepsilon_D|n\rangle\langle n| - \sum_{1\leqslant n,n+1\leqslant N} (V|n\rangle\langle n+1| + \text{H.c.}). \tag{A3}$$

For the infinite uniform chain $H_{-\infty\infty}$ with a section H_{1N}, the GF can be evaluated directly from Eq. (2),

$$g^I_{nn'} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{ik(n-n')}}{E+i\delta-(\epsilon_D-2V\cos k)} = \frac{e^{iq|n-n'|}}{2iV\sin q}, \quad n,n' \in Z, \tag{A4}$$

where the wave vector q is given in Eq. (16).

The semi-infinite chain $H_{1\infty}$ is a subsystem of $H_{-\infty\infty}$. By means of the lemma, its GF can be obtained as

$$g^{SI}_{nn'} = \frac{e^{iq|n-n'|} - e^{iq(n+n')}}{2iV\sin q}, \quad n,n' \geqslant 1. \tag{A5}$$

Finally, viewing H_{1N} as a subsystem of $H_{1\infty}$ and using the lemma again, we arrive at the GF of H_{1N},

$$g_{nn'} = \frac{\sin[(N+1-\max\{n,n'\})q]}{-V\sin[(N+1)q]} \frac{\sin(\min\{n,n'\}q)}{\sin q}, \quad 1 \leqslant n,n' \leqslant N. \tag{A6}$$

Some special cases have been given in the paper. The method used here can easily be generalized to the two-dimensional situation.

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[1] E. Scheer, N. Agraït, J. C. Cuevas, A. L. Yeyati, B. Ludoph, A. Martín-Rodero, G. R. Bollinger, J. M. van Ruitenbeek, and C. Urbina, Nature (London) **394**, 154 (1998).

[2] A. I. Yanson, G. Rubio-Bollinger, H. E. van den Brom, N. Agräït, and J. M. van Ruitenbeek, Nature (London) **395**, 783 (1998).

[3] H. Ohnishi, Y. Kondo, and K. Takayanagi, Nature (London) **395**, 780 (1998).

[4] H. S. Sim, H. W. Lee, and K. J. Chang, Phys. Rev. Lett. **87**, 096803 (2001).

[5] Z. Y. Zeng and F. Claro, Phys. Rev. B **65**, 193405 (2002).

[6] T. S. Kim and S. Hershfield, Phys. Rev. B **65**, 214526 (2002).

[7] R. H. M. Smit, C. Untiedt, G. Rubio-Bollinger, R. C. Segers, and J. M. van Ruitenbeek, Phys. Rev. Lett. **91**, 076805 (2003).
[8] P. A. Orellana, F. Domínguez-Adame, I. Gómez, and M. L. Ladrón de Guevara, Phys. Rev. B **67**, 085321 (2003).
[9] P. A. Orellana, M. L. Ladrón de Guevara, M. Pacheco, and A. Latgé, Phys. Rev. B **68**, 195321 (2003).
[10] F.-Q. Xie, L. Nittler, Ch. Obermair, and Th. Schimmel, Phys. Rev. Lett. **93**, 128303 (2004).
[11] G. Binnig and H. Rohrer, Rev. Mod. Phys. **71**, S324 (1999).
[12] A. Yacoby, M. Heiblum, D. Mahalu, and H. Shtrikman, Phys. Rev. Lett. **74**, 4047 (1995).
[13] R. Schuster, E. Buks, M. Heiblum, D. Mahalu, V. Umansky, and H. Shtrikman, Nature (London) **385**, 417 (1997).
[14] C. Bruder, R. Fazio, and H. Schoeller, Phys. Rev. Lett. **76**, 114 (1996).
[15] G. Hackenbroich, W. D. Heiss, and H. A. Weidenmüller, Phys. Rev. Lett. **79**, 127 (1997).
[16] P. G. Silvestrov and Y. Imry, Phys. Rev. Lett. **85**, 2565 (2000).
[17] R. Baltin and Y. Gefen, Phys. Rev. Lett. **83**, 5094 (1999).
[18] H. Xu and W. Sheng, Phys. Rev. B **57**, 11903 (1998).
[19] C. M. Ryu and S. Y. Cho, Phys. Rev. B **58**, 3572 (1998).
[20] T. Taniguchi and M. Büttiker, Phys. Rev. B **60**, 13814 (1999).
[21] H. W. Lee, Phys. Rev. Lett. **82**, 2358 (1999).
[22] A. L. Yeyati and M. Büttiker, Phys. Rev. B **62**, 7307 (2000).
[23] H. Q. Xu and B. Y. Gu, J. Phys.: Condens. Matter **13**, 3599 (2001).
[24] I. C. Fasth and H. Q. Xu, Physica A **17E**, 579 (2003).
[25] H. Q. Xu, I. C. Fasth, D. Csontos, L. B. Zhang, and Y. Zhao, Phys. Rev. B **68**, 241306(R) (2003).
[26] W. G. van der Wiel, S. De Franceschi, T. Fujisawa, J. M. Elzerman, S. Tarucha, and L. P. Kouwenhoven, Science **289**, 2105 (2000); Y. Ji, M. Heiblum, D. Sprinzak, D. Mahalu, and H. Shtrikman, *ibid.* **290**, 779 (2000); K. Kobayashi, H. Aikawa, S. Katsumoto, and Y. Iye, Phys. Rev. Lett. **88**, 256806 (2002).
[27] D. S. Fisher and P. A. Lee, Phys. Rev. B **23**, R6851 (1981).
[28] H. Q. Xu and W. D. Sheng, Superlattices Microstruct. **25**, 79 (1999).
[29] H. Q. Xu, Phys. Rev. B **66**, 165305 (2002).
[30] A. Aldea, P. Gartner, and I. Corcotoi, Phys. Rev. B **45**, 14122 (1992).
[31] F. Sols, M. Macucci, U. Ravaioli, and K. Hess, Appl. Phys. Lett. **54**, 350 (1989); F. Sols, M. Macucci, U. Ravaioli, and K. Hess, J. Appl. Phys. **66**, 3892 (1989); Zhi-an Shao, W. Porod, and C. S. Lent, Phys. Rev. B **49**, 7453 (1994); P. S. Deo and A. M. Jayannavar, *ibid.* **50**, 11629 (1994); M. Büttiker and C. A. Stafford, Phys. Rev. Lett. **76**, 495 (1996).
[32] M. Büttiker, Y. Imry, and M. Ya. Azbel, Phys. Rev. A **30**, 1982 (1984); Zhi-an Shao, W. Porod, and C. S. Lent, Appl. Phys. Lett. **61**, 1350 (1992).
[33] H. Tamura and T. Ando, Phys. Rev. B **44**, 1792 (1991).