Coherent transmission through a one dimensional lattice

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Abstract

Based on the Keldysh nonequilibrium Green function (NGF) technique, a general formula for the current and transmission coefficient through a one dimensional lattice is derived without the consideration of electron-electron interactions. We obtain an analytical condition for perfect resonant transmission when the levels of sites are aligned, which depends on the parity of the number of sites. Localization-delocalization transition in a generic one dimensional disordered lattice is also analyzed, depending on the correlation among the hopping parameters and the strength of the coupling to reservoirs. The dependence of the number and lineshape of resonant transmission and linear conductance peaks on the structure parameters of the lattice is also given in several site cases.
I. INTRODUCTION

Transport through a quantum dot lattice depends on the matching of electron levels in the various quantum dots\(^1\). If the electron levels of individual dots are aligned, resonant tunneling occurs\(^2\). Electronic transport through these structures is usually investigated theoretically on the basis of a "classic" rate equation in the weak coupling limit\(^3, 4\), and a quantum rate equation in the strong and weak coupling limits\(^1, 2\). The splitting due to the interdot coupling has also been calculated by Matveev et al.\(^5\) and Golden et al.\(^6\). Some groups have recently investigated in detail the spectral and current properties of a coupled quantum dot pair following the Keldysh nonequilibrium Green's function (NGF) formalism\(^7\). Calculations on Phonon-assisted\(^8\) and photon-assisted\(^9\) transport in two coupled quantum dots have been recently conducted, in which an electron pump effect is found. Kondo physics and other correlation effects in the same system have also been considered\(^10\). In quantum dot systems, electron-electron interaction becomes important and Coulomb oscillation of linear conductance and even Kondo effect arise\(^11, 12\). Experimentally, as early as 1990, Kouwenhoven et al.\(^13\) performed a transport experiment in a sample consisting of fifteen dots. Some experiments have also been conducted to explore the ground-state properties of a double quantum dot\(^14\). Very recently, Oosterkamp et al.\(^15\) investigated experimentally microwave spectroscopy of a two quantum dot molecule.

Recently electronic transport in metallic chains of single atoms has attracted both theoretical\(^16, 17\) and experimental\(^18\) interest, since atomic wires represent the ultimate limit of the miniaturization of electrical conductors. Although atomic wires are somewhat simple toy models in textbooks and literatures, they may be the best laboratory to test physical properties of one dimensional (1D) systems. The microscopic mechanism for the conductance quantization of atomic wires still keeps vague in spite of some endeavours\(^19\). First-principle calculations\(^16\) and analytical deduction\(^17\) demonstrated interesting oscillation of conduction of the monoatomic wires with the number of atoms, which was observed experimentally in the conductance of mechanically controllable break junctions atomic contacts\(^18\). The parity effect in the conductance was also found in weakly disordered quasi-1D tight-binding models\(^20\) and dirty superconducting wires\(^21\). However, whether the interesting parity phenomena arising from single particle behavior\(^17\) or many-body correlation effects\(^22\) need more clarifications.
To have a better understanding the transport properties of generic one dimensional systems and clarify conductance quantization in such a system, we consider electron transmission through a one dimensional lattice where the sites allow for only the nearest-neighboring hopping. The lattice is linked to reservoirs through the leads. Such a kind of lattice may be one dimensional quantum dot array or chains of atoms. In this work we adopt the Keldysh NGF formalism rather than other method such as classic or quantum rate equation, since the NGF prescription allows one to obtain explicitly analytical current and transmission formulas, which are valid in both the strong and weak coupling limits. We develop a technique to calculate the retarded Green functions for every site based on the equations-of-motion method. With the help of the technique we developed, it is very convenient and intuitive to calculate the retarded and correlation Green functions for every lattice sites. As the transmission and current formula is applied to the cases of a single and a double site structure, some well-known results are rediscovered, with some new phenomena being observed. The case of triple sites shows more complicated and interesting resonant transmission structure. If the lattice-lead couplings are asymmetric, the resonant structure of the transmission spectra for the triple site structure has weak dependence on the arrangement of site levels if they are not aligned. Moreover, we derive an analytical expression for the condition for perfect transmission of a one dimensional lattice. Such a condition depends on whether the number of sites is odd or even, suggesting that the parity feature of the linear conductance of a one dimensional system does not arise from the electron-electron correlation effects, since we did not consider electron-electron interactions. In the case of symmetric lattice-lead couplings, our result is consistent with the parity effect of conductance in monatomic wires based on the first-principles calculations \cite{16} and experimental findings \cite{18}.

We notice that Shangguan et al. \cite{23} studied the differential conductance and charge distribution in a linear quantum dot array based on the similar formalism. However, there exist some crucial discrepancies between our formalisms and results. First, the prescriptions for the calculation of the correlation Green functions such as less-than one are different. After repeating the use of the Keldysh formula in the noninteraction case with the help of the properties $G^r G^a = (G^r - G^a)/(2i Im G^a)$, we obtain finally the transmission formula (23), which is different formally from the result of Shangguan et al. \cite{23}, Eq. (27) in their paper, without using the mentioned property. Such a prescription is more intuitive and facilitates greatly the analysis of the dependence of transmission probability on the parameters of the
system especially at resonance, as can be seen in the N-site case. Second, we study the linear transport properties such as resonant transmission, linear conductance, while Shangguan et al. investigate the nonlinear ones such as differential conductance, charge distribution. We also extend the result to conductance quantization in monovalent atomic chains and the localization-delocalization transition in a generic one dimensional system, a fundamental issue in the condensed-matter physics.

The rest of the paper is organized as follows. In Sec. II we formulate the transport in a one dimensional lattice and derive the formulas for calculating the current, transmission and conductance based on the Keldysh NGF method. In Sec. III we use the formulas to calculate the transmission and conductance spectra for a single cite, a double site and a triple site structures, with a detailed analysis of our results. Also we derive an analytical expression for the condition for perfect transmission of N-site lattices as the site levels are aligned. Concluding remarks are given in Sec. IV.

II. MODEL AND FORMULATION

We are interested in the electronic transport properties of a one dimensional lattice with N sites. The lattice is connected to the left(right) lead L(R), which can be described by a tunneling matrix element. The leads are considered electron reservoirs with a continuum of states filled up to their respective Fermi levels \( \mu_L \) and \( \mu_R \) at zero temperature. Such a device can be described by a single-band tight-binding model. The on-site energy of site \( i \) is labelled by \( \epsilon_i \). An inter-site coupling with matrix element \( t_i \) accounts for the electron’s hopping between nearest-neighboring sites \( i \) and \( i + 1 \). The coupling between the left(right) lead \( L(R) \) and the first 1 (last \( N \)) site is described by a parameter \( v_{kL} (v_{kR}) \). Then a tight-binding Hamiltonian for the lattice in the absence of electron-electron interaction takes the following form

\[
H = \sum_{k,\alpha=L,R} \epsilon_{\alpha,\alpha} a_{k\alpha}^+ a_{k\alpha} + \sum_{i=1}^{N} \epsilon_i d_i^+ d_i + \sum_{i=1}^{N-1} \left( t_i d_i^+ d_{i+1} + t_i^* d_i d_{i+1}^+ \right) \\
+ \sum_k \left( v_{kL} a_{kL}^+ d_1 + v_{kL}^* d_1^+ a_{kL} \right) + \sum_k \left( v_{kR} a_{kR}^+ d_N + v_{kR}^* d_N^+ a_{kR} \right)
\]  

(1)

where \( a_{kL}(a_{kL}^+), a_{kR}(a_{kR}^+) \) and \( d_i(d_i^+) \) \( (i = 1, 2, ..., N) \) are the annihilation (creation) operators for an electron in the left lead, right leads and at site \( i \). In Eq. (1), the first term is the Hamiltonian for the leads, the second term is the Hamiltonian for uncoupled \( N \) sites, while
the third and last two terms describe the coupling between neatest-neighboring sites and the couplings between the lattice and the leads.

Following Ref. [12], the current through the lattice is the time evolution of the electron number $N_L(t) = \sum_k a_k^\dagger(t) a_k(t)$ in the left lead

$$J_L = -e < \dot{N}_L > = \frac{i e}{\hbar} < \{N_L, H\} > = \frac{2 e}{\hbar} \text{Re} \{ \sum_k v_{kL} G^<_{1,k}(t,t) \}, \quad (2)$$

where the less-than Green function $G^<_{1,k}(t,t') = i < a_k^\dagger(t') d_1(t) >$. With the help of Dyson’s equation, the less-than Green function $G^<_{1,k}(t,t')$ can be written as

$$G^<_{1,k}(t,t') = \int dt_1 v_{kL}^* \left[ G_r^{1,1}(tt_1) g^<_{kL}(t_1,t') + G^<_{11}(t,t_1) g^a_{kL}(t_1,t') \right]. \quad (3)$$

In Eq. (3), $G^<_{11}(t,t') = i < d^\dagger_1(t') d_1(t) >$, $G^r_{11}(t,t') = -i \theta(t-t') < \{ d_1(t), d^\dagger_1(t') \} >$ are the less-than and retarded Green functions of electrons at site 1, while $g^a_{kL}(t,t')$ is the exact advanced (less-than) Green function of electrons in the left lead decoupled from the lattice

$$g^a_{kL}(t,t') = \mp i \theta(\pm t \mp t') e^{-i(\epsilon_{kL} - \mu_L)(t-t')}, \quad g^<_{kL}(t,t') = i f_L(\epsilon_{kL} - \mu_L) e^{-i(\epsilon_{kL} - \mu_L)(t-t')}.$$

Here $f_\alpha(x) = [\exp(x/k_B T) + 1]^{-1}$ ($\alpha = L, R$) is the Fermi-Dirac distribution function of the Lead. Substituting Eq. (3) into Eq. (2), changing the sum over $k$ into an integral $\int d\epsilon \rho_L(\epsilon)$ (where $\rho_L(\epsilon)$ the density of states in the left lead) and introducing a linewidth function $\Gamma_L(\epsilon) = 2\pi |v_{kL}|^2 \rho_L(\epsilon)$, we get a compact form of current formula in Fourier space

$$J_L = \frac{i e}{\hbar} \int \frac{d\epsilon}{2\pi} \Gamma_L(\epsilon) \left\{ f_L(\epsilon - \mu_L)[G^r_{11}(\epsilon) - G^a_{11}(\epsilon)] + G^<_{11}(\epsilon) \right\} \quad (4)$$

Now we turn to calculate the retarded (advanced) Green function $G^r_{11}(\epsilon)$ and the less-than Green function $G^<_{11}(\epsilon)$ of site 1. The essential idea to solve the retarded Green function is that we consider first site 2 neighboring to site 1 as a part of the right lead, and then consider site $i + 1$ as a part of the right lead when calculating the Green functions of site $i$. This procedure may be regarded as an extension of the well-known recursion or decimation method for calculating Green function [24]. From Dyson’s equation $G = (g^{-1} - \Sigma)^{-1}$, $G^r_{11}(\epsilon)$ can be written as

$$G^r_{11}(\epsilon) = [g^r_{11}(\epsilon)^{-1} - \Sigma^r_{11}(\epsilon)]^{-1}, \quad (5)$$
where \( g_{11}(\epsilon) \) is the retarded Green function of site 1 decoupled with the system, and

\[
\Sigma_{11}(\epsilon) = \Sigma_L(\epsilon) + \Sigma_{1R}(\epsilon),
\]

\[
\Sigma_L(\epsilon) = \sum_k |v_{kL}|^2 g_{kL}(\epsilon) = \Lambda_L(\epsilon) - \frac{i}{2}\Gamma_L(\epsilon),
\]

\[
\Sigma_{1R}(\epsilon) = |t_1|^2 G_{2R}(\epsilon).
\]  

\[
G_{2R}(\epsilon) \quad \text{(6)}
\]

\[
\Sigma_{11}(\epsilon) = \Sigma_L(\epsilon) + \Sigma_{1R}(\epsilon) = \Lambda_L(\epsilon) - \frac{i}{2}\Gamma_L(\epsilon) - |t_1|^2 G_{3R}(\epsilon).
\]  

\[
\Sigma_{1R}(\epsilon) = |t_1|^2 G_{2R}(\epsilon).
\]  

\[
G_{2R}(\epsilon) \quad \text{(7)}
\]

\[
\Sigma_{11}(\epsilon) = \Sigma_L(\epsilon) + \Sigma_{1R}(\epsilon) = \Lambda_L(\epsilon) - \frac{i}{2}\Gamma_L(\epsilon) - |t_1|^2 G_{3R}(\epsilon).
\]  

\[
\Sigma_{1R}(\epsilon) = |t_1|^2 G_{2R}(\epsilon).
\]  

\[
G_{2R}(\epsilon) \quad \text{(8)}
\]

\[
G_{2R}(\epsilon) = \left[ g_{22}(\epsilon) - \Sigma_{2R}(\epsilon) \right]^{-1},
\]  

\[
\Sigma_{2R}(\epsilon) = |t_2|^2 G_{3R}(\epsilon).
\]  

\[
G_{2R}(\epsilon) \quad \text{(9)}
\]

\[
G_{iR}(\epsilon) = \left[ g_{ii}(\epsilon) - \Sigma_{i+1R}(\epsilon) \right]^{-1},
\]

\[
\Sigma_{iR}(\epsilon) = |t_i|^2 G_{i+1R}(\epsilon).
\]  

\[
G_{iR}(\epsilon) \quad \text{(10)}
\]

Note that for the last site \( N \), its retarded Green function reads as

\[
G_{NR}(\epsilon) = \left[ g_{NN}(\epsilon) - \Sigma_{NR}(\epsilon) \right]^{-1},
\]

\[
\Sigma_{NR}(\epsilon) = \sum_k |v_{kR}|^2 g_{kR}(\epsilon) = \Lambda_R(\epsilon) - \frac{i}{2}\Gamma_R(\epsilon).
\]  

\[
G_{NR}(\epsilon) \quad \text{(11)}
\]

\[
G_{iR}(\epsilon) = \left[ g_{ii}(\epsilon) - \Sigma_{i+1R}(\epsilon) \right]^{-1},
\]

\[
\Sigma_{iR}(\epsilon) = |t_i|^2 G_{i+1R}(\epsilon).
\]  

\[
G_{iR}(\epsilon) \quad \text{(12)}
\]

Once the retarded and advanced Green functions are known (\( G^a = (G^r)^* \)), the less-than Green function can be evaluated with the help of the Keldysh formula for the present problem

\[
G^< = G^r \Sigma^< G^a = \frac{G^r - G^a}{1/G^a - 1/G^r} \Sigma^<.
\]  

\[
G^< \quad \text{(13)}
\]

Then

\[
G_{11}^< = \frac{G_{11}^r - G_{11}^a}{1/G_{11}^a - 1/G_{11}^r} \Sigma_{11}^<,
\]  

\[
G_{iR}^< = \frac{G_{iR}^r - G_{iR}^a}{1/G_{iR}^a - 1/G_{iR}^r} \Sigma_{iR}^<,
\]  

\[
G_{NR}^< = \frac{G_{NR}^r - G_{NR}^a}{1/G_{NR}^a - 1/G_{NR}^r} \Sigma_{NR}^<.
\]  

\[
G_{11}^< \quad \text{(14)}
\]

\[
G_{iR}^< \quad \text{(15)}
\]

\[
G_{NR}^< \quad \text{(16)}
\]
where the self energies are given by

\[ \Sigma_{11}^\le = \Sigma_L^\le + \Sigma_{1R}^\le = \Sigma_k \mid v_{kL} \mid^2 g_{kL}^\le(\epsilon) + \mid t_1 \mid^2 G_{2R}^\le(\epsilon), \]

\[ \Sigma_{1R}^\le = \mid t_i \mid^2 G_{i+1R}^\le(\epsilon), \]

\[ \Sigma_R^\le = \Sigma_k \mid v_{kL} \mid^2 g_{kL}^\le(\epsilon) = if_R(\epsilon - \mu_R)\Gamma_R. \]

Since \( \frac{1}{G^a} - \frac{1}{G^r} = \Sigma^r - \Sigma^a \), combining Eqs. (14) – (16) yields

\[ G_{11}^\le(\epsilon) = -\frac{f_L(\epsilon - \mu_L)\Gamma_L + f_R(\epsilon - \mu_R)\Gamma_2}{\Gamma_L + \Gamma_2}[G_{11}^r(\epsilon) - G_{11}^a(\epsilon)], \]

where \( \Gamma_2 = i \mid t_1 \mid^2 [G_{2R}^r(\epsilon) - G_{2R}^a(\epsilon)] = -2\mid t_1 \mid^2 ImG_{2R}^r \). Substituting the above expression into the current formula (4), one obtains the following Landauer-Büttiker-type formula

\[ J_L = -\frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi}[f_L(\epsilon - \mu_L) - f_R(\epsilon - \mu_R)] \frac{\Gamma_L \Gamma_2}{\Gamma_L + \Gamma_2} ImG_{11}^r(\epsilon). \]

Equation (22) is the central result of this work. This formula for steady transport is valid both in the strong and weak coupling limits. It is also applicable to the nonequilibrium situation. In Eq. (22), the term

\[ T(\epsilon) = -\frac{2\Gamma_L \Gamma_2}{\Gamma_L + \Gamma_2} ImG_{11}^r(\epsilon), \]

is the transmission coefficient for electron tunneling through the one-dimensional lattice. Furthermore, the differential conductance \( \mathcal{G} \) in the linear regime \( \mu_L - \mu_R \to 0^+ \) can be readily derived as

\[ \mathcal{G} = -\frac{e^2}{\hbar} \int d\epsilon T(\epsilon) \frac{\partial f(\epsilon - \mu_L)}{\partial(\epsilon)} \]

It is noted that the above procedure to calculate the related Green functions can be extended to two and three dimensional lattices with each site having multiple levels in the presence of electron-electron interactions treated in the mean-field approximation, which will be published elsewhere. In addition, such a procedure is very suitable to numerical calculation of the spectral density and tunneling quantities in coupled many site systems.

III. TRANSMISSION AND CONDUCTANCE

In this section we will investigate coherent transmission and conductance in a one dimensional lattice, which may be related to a one dimensional quantum dot/well array or a chain
of single atoms. Our interest is mainly to find out how parameters determine the number and position of resonant transmission and conductance peaks.

A. Single site

In the case of single site, the Green function and self-energy take the following simple form

\[
G_{11}^r(\epsilon) = (\epsilon - \epsilon_1 - \Lambda + \frac{i}{2}\Gamma)^{-1},
\]

\[
\Gamma_2 = \Gamma_R,
\]

(25)

where \(\Lambda = \Lambda_L + \Lambda_R, \Gamma = \Gamma_L + \Gamma_R\). Then the transmission and conductance are

\[
\mathcal{T}(\epsilon) = \frac{\Gamma_L \Gamma_R \mathcal{F}_1(\epsilon)}{\epsilon_1 + \Lambda - \epsilon \mu_L + i\Gamma/2}
\]

\[
\mathcal{G} = \frac{e^2 \Gamma_L \Gamma_R}{\hbar \Gamma} \left[ \epsilon_1 + \Lambda - \epsilon \mu_L + i\Gamma/2 \right]
\]

\[
+ \frac{1}{4\pi^3 k_B T} \sum_{\eta = \pm} \text{Re} \Psi^{(1)} \left( \frac{1}{2} + \frac{\eta \Gamma}{4\pi k_B T} + \frac{i \epsilon_1 + \Lambda - \epsilon \mu_L}{2\pi k_B T} \right),
\]

(26)

where \(\mathcal{F}_1(\epsilon) = [(\epsilon - \epsilon_1 - \Lambda)^2 + (\Gamma_L + \Gamma_R)^2/4]^{-1}\), and \(\Psi^{(1)}\) is the trigamma function [25]. It is obvious that the transmission coefficient is of the Breit-Wigner type. Only if the coupling between the site and the two leads is symmetric, i.e., \(\Gamma_L = \Gamma_R\), perfect resonant transmission (\(\mathcal{T} = 1\)) can occur at the renormalized dotsite level \(\epsilon_1 + \Lambda\), while for asymmetric coupling \(\Gamma_L \neq \Gamma_R\), the transmission coefficient \(\mathcal{T}\) is always less than 1. The larger the asymmetry, the smaller the transmission coefficient. Thus conductance quantization can be achieved for the 1-site system in the symmetric lattice-lead coupling case.

B. Double sites

In the case of two coupled sites, it is expected that the competition between the coupling of the sites and the sites and leads play a crucial role on the transmission and conductance. In the absence of coupling to the leads, the level associated with two equal sites will split into two levels due to the coupling between them. The separation between these two split levels is proportional to the coupling strength. When the sites are connected to the leads, one should consider the sites and the leads as a single system, with the result that now the size of the level splitting depends on both the couplings between sites and leads.
Consider first a double site structure without coupling to the leads. Assuming the coupling strength between these two sites is \( t \), the hamiltonian becomes \( \epsilon_1 d_1^+ d_1 + \epsilon_2 d_2^+ d_2 + t d_1^+ d_2 + t^* d_2^+ d_1 \). Then the retarded Green functions for the two sites are

\[
G_{1r}(\epsilon) = \frac{1}{\epsilon - \epsilon_1 - i \epsilon_1^0 + |t|^2/(\epsilon - \epsilon_2 - i \epsilon_2^0)},
\]

\[
G_{2r}(\epsilon) = \frac{1}{\epsilon - \epsilon_2 - i \epsilon_2^0 - |t|^2/(\epsilon - \epsilon_1 - i \epsilon_1^0)}.
\]

One can readily find that the above two retarded Green functions have the same two poles at

\[
\epsilon = \frac{\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4|t|^2}}{2}.
\]

Note that when \( \epsilon_1 = \epsilon_2 \), the level separation is simply \( 2|t| \). The above analysis clearly shows that the larger the coupling, the bigger the separation between the two split levels. When the sites are connected to the two leads, this new coupling may modify the effective coupling between the sites as will be discussed in what follows.

The associated retarded Green functions in the presence of coupling with the two leads read

\[
G_{11r}(\epsilon) = [\epsilon - \epsilon_1 - \Lambda_L + \frac{i}{2} \Gamma_L - |t|^2 G_{2R}^r(\epsilon)]^{-1},
\]

\[
G_{2R}^r(\epsilon) = (\epsilon - \epsilon_2 - \Lambda_R + \frac{i}{2} \Gamma_R)^{-1},
\]

and

\[
\Gamma_2 = \Gamma_R |t|^2 / B(\epsilon),
\]

where \( B(\epsilon) = (\epsilon - \epsilon_2 - \Lambda_R)^2 + \Gamma_R^2/4 \). Substituting Eqs. (29)-(31) into the expression (23) yields

\[
\mathcal{T}(\epsilon) = \Gamma_L \Gamma_R |t|^2 \mathcal{F}_2(\epsilon)
\]

where

\[
\mathcal{F}_2(\epsilon) = \frac{B(\epsilon)}{[\epsilon - \epsilon_1 - \Lambda_L]B(\epsilon) - |t|^2 (\epsilon - \epsilon_2 - \Lambda_R)^2 + [\Gamma_L B(\epsilon) + |t|^2 \Gamma_R ]^2 / 4}.
\]

We now consider the case when the levels of the isolated sites 1 and 2 are the same \( (\epsilon_1 = \epsilon_2 = \epsilon_0) \). In the case of symmetric coupling, i.e., \( \Gamma_L = \Gamma_R = \Gamma, \Lambda_L = \Lambda_R = \Lambda \), the condition for perfect resonant transmission is that

\[
(\epsilon - \epsilon_0 - \Lambda)^2 + \Gamma^2/4 = |t|^2
\]
has real roots. This equation also determines the number and position of the resonant transmission peaks. Obviously, the condition for perfect resonant transmission is $|t|^2 \geq \Gamma^2/4$. There will be then only one perfect resonant transmission peak located at $\epsilon = \epsilon + \Lambda$ when $|t|^2 = \Gamma^2/4$. If $|t|^2 \leq \Gamma^2/4$, there is just one imperfect resonant peak ($T < 1$) pinned at $\epsilon = \epsilon_0 + \Lambda$. In the case of $|t|^2 > \Gamma^2/4$, two perfect transmission peaks exist at $\epsilon_{\pm} = \epsilon_0 + \Lambda \pm \sqrt{|t|^2 - \Gamma^2/4}$. These features can be clearly seen in Fig. 1 (a), where we can also appreciate that the lineshape of all the transmission peaks is Lorenzian. Here and in all figures following energies are in arbitrary units.

Next we consider what would happen if the coupling between the sites and the two leads becomes asymmetric. In this case, one can find from the expression of the transmission coefficient (32) that the condition for perfect transmission is $|t|^2 = \Gamma_L \Gamma_R/4$ and only one perfect transmission peak can be expected at $\epsilon = \epsilon_0 + \Lambda$. In all other cases, the transmission coefficient is less than 1. In Fig. 1 (b) we show the transmission coefficient for various inter-site coupling constants $t$ for $\Gamma_L = 0.25$ and $\Gamma_R = 4$. If the level shift $\Lambda_L$ and $\Lambda_R$ induced by the left and right lead are not the same, the lineshape of the transmission peaks is non-Lorenzian, as is apparent in the case $\Lambda_L = 0.025$, $\Lambda_R = 0.4$ also shown in the figure. Figure 1 (c) and (d) are the plots of the transmission coefficient for increasing inter-site coupling $t$ in the symmetric and asymmetric coupling cases, respectively. When the levels of the sites are not aligned. It is then expected that no perfect resonant transmission exists. One can observe that two symmetric transmission peaks always resolved in the symmetric coupling case. As the inter-site coupling $t$ increases, the maximum value as well as the separation of the transmission peaks increases. For asymmetric coupling, one transmission peak can be expected when the coupling between the sites is weak, and two asymmetric transmission peaks when it is strong. In addition, with increasing interdot coupling $t$, the value of the transmission coefficient increases first and then decreases after it is saturated. The position of the principal transmission peak is closer to the level of the site with smaller coupling to the lead.

This complex behavior reflects the competition between two resonances derived from the ground state of each site when far apart. As they come together and when coupling increases, the resonances approach the ground and first excited states of the compound system, which in general separated in energy. If the coupling is weak, on the other hand, the peaks will only be resolved if their width is smaller than the energy difference $\Delta \epsilon = |\epsilon_2 - \epsilon_1|$. If the
couplings to the leads is asymmetric the competing resonances will be dominated by that whose associated wavefunction is concentrated on the site region must weakly coupled to the lead.

To sum up, we have investigated in detail the resonant structure of the transmission coefficient of a coupled double site structure in the linear regime. We found that when the levels of the two sites are aligned, the condition for perfect resonant transmission is $|t|^2 \geq \Gamma^2/4$ in the case of symmetric site-lead coupling, and $|t|^2 = \Gamma_L \Gamma_R/4$ in the asymmetric case, which is consistent with the derivations of Ref. [27]. Once there exists a mismatch between the two levels of the sites, no perfect resonant transmission peak can be expected. In the case of symmetric site-lead coupling, the value of the transmission coefficient increases with increasing inter-site coupling, until it is saturated. For asymmetric site-lead coupling, the transmission coefficient increases first and then decreases after it reaches a maximum, as the inter-site coupling is increased. Moreover, in the asymmetric case, the splitting of the transmission peak requires a stronger inter-site coupling $t$. Asymmetry between the two split transmission peaks can be observed when the two levels are not aligned for asymmetric site-lead coupling, provided the inter-site coupling is strong enough. In addition, different level shifts of the two sites induced by the coupling to the leads will introduce a non Lorenzian lineshape of the transmission peak(s). The results imply that no perfect transmission and then no conductance quantization can be expected for double site systems in the symmetric coupling case (inversion symmetry).

C. Triple Sites

A coupled triple site structure is expected to contain richer physics than a coupled double site system, since it permits more interesting arrangement of the energy levels in each site and the competition between inter-site couplings. Surprisingly, electronic transport through the triple sites has been less investigated in the past both theoretically and experimentally [28]. In this subsection, we study the detailed dependence of the number and profile of transmission peaks, on the parameters of such a structure.

For an isolated triple site system, the hamiltonian can be written as

$$H = \epsilon_1 d_1^+ d_1 + \epsilon_2 d_2^+ d_2 + \epsilon_3 d_3^+ d_3 + t_L d_1^+ d_2 + t_L^* d_2^+ d_1 + t_R d_2^+ d_3 + t_R^* d_3^+ d_2,$$  (35)
where \( t_L \) and \( t_R \) are the couplings between sites 1 and 2, and 2 and 3, respectively. The related retarded Green functions are readily derived as

\[
G^r_1(\epsilon) = \frac{1}{\epsilon - \epsilon_1 - i0^+ - \frac{|t_L|^2}{\epsilon - \epsilon_2 - i0^+ - \frac{|t_R|^2}{\epsilon - \epsilon_3 - i0^+}}},
\]

\[
G^r_2(\epsilon) = \frac{1}{\epsilon - \epsilon_2 - i0^+ - |t_L|^2/(\epsilon - \epsilon_1 - i0^+) - |t_R|^2/(\epsilon - \epsilon_3 - i0^+)},
\]

\[
G^r_3(\epsilon) = \frac{1}{\epsilon - \epsilon_3 - i0^+ - \frac{|t_R|^2}{\epsilon - \epsilon_2 - i0^+ - \frac{|t_L|^2}{\epsilon - \epsilon_1 - i0^+}}},
\]

(36)

when the levels of three sites are aligned, i.e., \( \epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_0 \), each of these three retarded Green functions has the same three poles at \( \epsilon = \epsilon_0 \), \( \epsilon = \epsilon_0 + \sqrt{|t_L|^2 + |t_R|^2} \) and \( \epsilon = \epsilon_0 - \sqrt{|t_L|^2 + |t_R|^2} \). When the three electron levels are mismatched, there exist in general three poles in the above retarded Green functions, that is to say, the position of the original levels are moved due to the existence of the inter-site couplings. As the couplings between the structure and the leads are turned on, the Green functions for calculating the transmission coefficient become

\[
G^r_{11}(\epsilon) = [\epsilon - \epsilon_1 - \Lambda_L + \frac{i}{2}\Gamma_L - |t_L|^2G^r_{2R}(\epsilon)]^{-1},
\]

(37)

\[
G^r_{2R}(\epsilon) = (\epsilon - \epsilon_2 - |t_R|^2G^r_{3R})^{-1},
\]

(38)

\[
G^r_{3R}(\epsilon) = (\epsilon - \epsilon_3 - \Lambda_R + \frac{i}{2}\Gamma_R)^{-1},
\]

(39)

and

\[
\Gamma_2 = -2|t_L|^2ImG^r_{2R}.
\]

(40)

Then the transmission coefficient becomes

\[
\mathcal{T}(\epsilon) = \Gamma_L\Gamma_R|t_L|^2|t_R|^2\mathcal{F}_3(\epsilon),
\]

(41)

where

\[
\mathcal{F}_3(\epsilon) = \frac{B(\epsilon)}{C(\epsilon)[(\epsilon - \epsilon_1 - \Lambda_L - |t_L|^2ReG^r_{2R})^2 + (\Gamma_L - 2|t_L|^2ImG^r_{2R})^2/4]}
\]

(42)

with

\[
B(\epsilon) = (\epsilon - \epsilon_3 - \Lambda_R)^2 + \frac{\Gamma_R^2}{4},
\]

\[
C(\epsilon) = [((\epsilon - \epsilon_2)B(\epsilon) - |t_R|^2(\epsilon - \epsilon_3 - \Lambda_R))^2 + |t_R|^4\frac{\Gamma_R^2}{4},
\]
and
\[
ReG_{2R}^\sigma(\epsilon) = \frac{1}{2} \left[ \frac{(\epsilon - \epsilon_2) B(\epsilon) - |t_R|^2 (\epsilon - \epsilon_3 - \Lambda_R)}{C(\epsilon)} B(\epsilon) \right],
\]
\[
ImG_{2R}^\sigma(\epsilon) = -\frac{|t_R|^2 \Gamma_R B(\epsilon)}{C(\epsilon)}.
\]
(43)

Now we consider the case when the three levels of sites are aligned and neglect the energy shifts \(\Lambda_L\) and \(\Lambda_R\). At resonance \(\epsilon = \epsilon_0\), one has
\[
B(\epsilon) = \frac{\Gamma_R^2}{4},
\]
\[
C(\epsilon) = |t_R|^4 \frac{\Gamma_R^2}{4},
\]
\[
ImG_{2R}^\sigma(\epsilon) = -\frac{\Gamma_R}{2|t_R|^2},
\]
(44)

then one can easily derive the condition for perfect transmission
\[
|\frac{t_L}{t_R}|^2 = \frac{\Gamma_L}{\Gamma_R}.
\]
(45)

Further analytical results in this case are cumbersome, so we shall next provide some numerical results on the transmission spectra of the coupled triple site structure in various cases. Figures 2 and 3 show the transmission spectra for symmetric coupling \((\Gamma_L = \Gamma_R = 1)\), and asymmetric coupling \((\Gamma_L = 1, \Gamma_R = 4)\) to the left and right leads, respectively. In the figures four kinds of arrangements of energy levels are presented: (a) aligned levels \(\epsilon_1 = \epsilon_2 = \epsilon_3 = 10\), (b) ladder levels \(\epsilon_1 = 9, \epsilon_2 = 10, \epsilon_3 = 11\), (c) V-type levels \(\epsilon_1 = 9, \epsilon_2 = 11, \epsilon_3 = 9\) and (d) two aligned neighboring levels \(\epsilon_1 = 9, \epsilon_2 = 9, \epsilon_3 = 11\). From Fig. 2 (a), one finds that there exists only one perfect transmission peak located at \(\epsilon = \epsilon_0\) when the inter-site couplings are equal and small. As \(t_L = t_R\) are increased, the perfect transmission peak splits symmetrically. Once the energy shifts are taken into consideration, the transmission peaks are no longer equally spaced (dotted line in Fig. 2 (a)). Since Eq. (45) is no longer satisfied, there is no perfect transmission when \(t_L \neq t_R\).

In the case of levels arranged in a ladder sequence (Fig. 2 (b)), one perfect transmission peak with two low shoulders is obtained for \(t_L = t_R = 0.5\). As they both reach the value 2, the shoulders become two imperfect transmission peaks and the perfect transmission peak at the center is widened. When the inter-site couplings are not equal, the transmission peaks are suppressed and arranged into a ladder type. When the three site levels are in the V-type disposition, interesting transmission spectra are observed. If the inter-site couplings are
equal and small, one sharp perfect transmission peak and one broad imperfect transmission peak are seen. As the inter-site couplings increase, the imperfect transmission peak splits and the resonances move further apart. Similarly, the inequality of $t_L$ and $t_R$ decreases the transmission in all three peaks. In fact the value of the transmission coefficient through split electron levels is determined by the extension to the leads of the wavefunctions for these split electron levels. Then the above phenomena can be similarly explained as we did in the case of two coupled sites. Figure 2 (d) shows the transmission spectra for $\epsilon_1 = 9$, $\epsilon_2 = 9$, $\epsilon_3 = 11$. One can see two asymmetric imperfect transmission peaks as $t_L = t_R = 0.5$. When they reach the value 2, three imperfect transmission peaks of different height are discerned. As in the case of three ladder levels, the asymmetry between two inter-site couplings $t_L$ and $t_R$ rearranges these three transmission peaks into a ladder. Notice that no perfect transmission peak even appears in this case.

Now we investigate how the transmission spectra are modified when the site-lead couplings are asymmetric. One can find from Fig. 3 that perfect transmission exists only in the case of three aligned levels under the condition for perfect transmission. Figure 3 (a) is the transmission spectra for different inter-site couplings when the levels of three sites are aligned. One imperfect transmission peak is seen as $t_L = t_R$ and one perfect transmission peak along with two narrow shoulders is observed as $t_L = 1$, $t_R = 2$, which satisfies the condition for perfect transmission (45). Also one can find different resonant structures for the cases $|t_L/t_R|^2 > \Gamma_L/\Gamma_R$ and $|t_L/t_R|^2 \leq \Gamma_L/\Gamma_R$. When the three levels are not aligned, no perfect transmission occurs in the case of asymmetric site-lead couplings, which is demonstrated in Fig. 3 (b)-(d). The transmission spectra in the case of levels arranged in a ladder exhibit one imperfect transmission peak and one shoulder structure as $t_L = t_R = 0.5$. Increasing the inter-site couplings, the shoulder becomes gradually distinguished as a transmission peak. The competition between $t_L$ and $t_R$ strongly modifies the resonant structure of the transmission spectra. Comparing Fig. 3 (b)-(d), one may find that the resonant structure of the transmission spectra are similar and mainly display two transmission peaks structure. It suggests a fact that, as the site-lead couplings are not symmetric, the resonant structure of the transmission spectra has weak dependence on the arrangement of the electron levels of sites if they are not aligned.

From the above analysis, the transmission spectra of three coupled sites is more complicated and contains more physics than that of two coupled sites. The main features of the
transmission spectra for a triple site structure are as follows: (1) the transmission spectra may contain just one, two or three resonant peaks, (2) the resonant structure of the transmission spectra is strongly dependent on the arrangement of the electronic levels when the site-lead couplings are symmetric, while weak dependence on the arrangement of the electron levels if they are not, (3) the resonant structure of the transmission spectrum strongly depends on the symmetry between inter-site couplings, (4) perfect transmission and thus conductance quantization can be achieved for a triple site system with inversion symmetry when coupled symmetrically to reservoirs. These conclusions hold for the linear conductance \( G \) as well, since the conductance and the transmission coefficient possess the same resonant structure at low temperatures. Our theoretical results are consistent with the experiment observations in the conductance of triple sites [28].

D. N Sites

As can be found from our previous analysis, the condition for perfect transmission is different for one, two and three site structures. It gives us a hint that the condition for perfect transmission would depend on whether the number of sites in a 1D lattice is even or odd. In what follows, we derive the condition under which the perfect transmission happens when the electron levels of the lattice are aligned and energy shifts are ignored, i.e., \( \epsilon_1 = \epsilon_2 = \cdots = \epsilon_N = \epsilon_0 \), and \( \Lambda_L = \Lambda_R = 0 \). From the expression for the transmission coefficient (23) and for \( \Gamma_2 \), one has

\[
T(\epsilon) = \frac{4\Gamma_L |t_1|^2 ImG_{2R}^r ImG_{11}^r(\epsilon)}{\Gamma_L - 2|t_1|^2 ImG_{2R}^r} = \frac{-2\Gamma_L |t_1|^2 ImG_{2R}^r}{(\epsilon - \epsilon_0 - |t_1|^2 ReG_{2R}^r)^2 + (\Gamma_L - 2|t_1|^2 ImG_{2R}^r)^2 / 4}. \tag{46}
\]

At resonance \( \epsilon = \epsilon_0 \), the real part of all the retarded Green functions becomes zero. Then the transmission coefficient is given by

\[
T = \frac{-8\Gamma_L |t_1|^2 ImG_{2R}^r}{(\Gamma_L - 2|t_1|^2 ImG_{2R}^r)^2}. \tag{47}
\]

Perfect transmission through the lattice, \( T = 1 \), is obtained if

\[
\Gamma_L = -2|t_1|^2 ImG_{2R}^r. \tag{48}
\]
Notice that since $g^0_i = 0$ ($i = 2, 3, \cdots N$) at resonance $\epsilon = \epsilon_0$, one can obtain the following expression for $\text{Im}G_{2R}^r$

$$\text{Im}G_{2R}^r = -\frac{\Gamma_R}{2} \frac{|t_3 t_5 \cdots t_{N-2}|^2}{t_2 t_4 \cdots t_{N-1}}; \quad N \text{ odd}$$

(49)

$$\text{Im}G_{2R}^r = -\frac{2}{\Gamma_R} \frac{|t_3 t_5 \cdots t_{N-1}|^2}{t_2 t_4 \cdots t_{N-2}}; \quad N \text{ even.}$$

(50)

Then the condition for perfect transmission is

$$\left| \frac{t_1 t_3 \cdots t_{N-2}}{t_2 t_4 \cdots t_{N-1}} \right|^2 = \frac{\Gamma_L}{\Gamma_R}; \quad N \text{ odd}$$

(51)

$$\left| \frac{t_1 t_3 \cdots t_{N-1}}{t_2 t_4 \cdots t_{N-2}} \right|^2 = \frac{\Gamma_L \Gamma_R}{4}; \quad N \text{ even.}$$

(52)

If the interdot couplings are the same, the condition becomes

$$\Gamma_L = \Gamma_R; \quad N \text{ odd}$$

(53)

$$|t_\pm|^2 = \frac{\Gamma_L \Gamma_R}{4}; \quad N \text{ even.}$$

(54)

Thus one can conclude that for a one dimensional lattice, the condition for perfect transmission is dependent on the parity of the sites of the lattice, i.e., whether the number of sites is odd or even. Equation (51) suggests that for a chain with an odd number of sites and inversion symmetry (i.e., $\Gamma^L = \Gamma^R = \Gamma, t_1 = t_{N-1}, t_2 = t_{N-2}, \text{ etc.}$) perfect transmission will be automatically satisfied at the middle of the band or level group. Thus the linear conductance is quantized to the value $2e^2/h$. This is not the case when $N$ is even. From the Eqs. (52) and (46), we find a transmission coefficient $4\eta/(1 + \eta)^2$ with $\eta = |\frac{2t_1 t_3 \cdots t_{N-1}}{t_2 t_4 \cdots t_{N-2}}|^2$ less than unity and a conductance smaller than $2e^2/h$. The even-odd feature appears in transmission and conductance in the absence of any electron interactions, thus the parity feature is not due to many particle effects. Our argument also proves that when the system is symmetric under inversion, the state at the middle of the band is always delocalized, regardless of the amount of disorder that respects such symmetry condition. Eqs. (51) and (52) defines a broad class of correlations in the disorder yielding delocalization of 1D disordered systems. This parity effect of conductance is consistent with the predictions in the monatomic wires based on the first-principles calculation\[16\] and confirmed by the experimental observations\[18\].

The dependence of transmission or conductance on the number of sites can be explained qualitatively as follows. To simplify our discussion, we constrain ourselves to the case when the inter-site couplings are the same, which corresponds to the monovalent atomic wire
When the number $N$ of sites is odd, one finds that the current through the middle site $(N + 1)/2$ can be written as

$$J_o = -\frac{2e}{\hbar} \int \frac{de}{2\pi} [f_L(\epsilon - \mu'_L) - f_R(\epsilon - \mu'_R)] \frac{\Gamma_{LD}\Gamma_{RD}ImG_{N-1/2}^r(\epsilon)}{\Gamma_{LD} + \Gamma_{RD}ImG_{N-1/2}^r(\epsilon)}, \quad (55)$$

where $\Gamma_{LD} = -2t^2ImG_{N-1/2}^r$ and $\Gamma_{RD} = -2t^2ImG_{N+1/2}^r$, with $G_{N-1/2}^L$ and $G_{N+1/2}^R$ are the Green’s functions decoupled from the middle site $(N + 1)/2$. In Eq. (55) we denote the chemical potential of the site left(right) to the middle site by $\mu'_L$($\mu'_R$) which equals to the chemical potential $\mu_L$($\mu_R$) in the equilibrium. The conductance at resonance can then be expressed as

$$G_o = \frac{2e^2}{h} \frac{4\Gamma_{LD}\Gamma_{RD}}{4(\Gamma_{LD} + \Gamma_{RD})^2}. \quad (56)$$

Obviously, the conductance reaches $\frac{2e^2}{h}$ only if $\Gamma_{LD} = \Gamma_{RD}$, which implies $\Gamma_L = \Gamma_R$ from the expressions of $\Gamma_{LD}$ and $\Gamma_{RD}$. When the site number $N$ is even, one can divide the lattice into two parts and then the current from the site $N/2$ to $(N + 2)/2$ can be written as

$$J_e = \frac{2e}{\hbar} \int \frac{de}{2\pi} [f_L(\epsilon - \mu'_L) - f_R(\epsilon - \mu'_R)] \frac{4t^2ImG_{N/2}^r L ImG_{N+2/2}^r R}{|1 - t^2G_{N/2}^r L G_{N+2/2}^r R|^2}. \quad (57)$$

The conductance at resonance ($ReG^r = 0$) is

$$G_e = \frac{2e^2}{h} \frac{4t^2ImG_{N/2}^r L ImG_{N+2/2}^r R}{|1 + t^2ImG_{N/2}^r L ImG_{N+2/2}^r R|^2}. \quad (58)$$

If $G_e = \frac{2e^2}{h}$, one needs $t^2 = (ImG_{N/2}^r L ImG_{N+2/2}^r R)^{-1}$, which eventually yields $t^2 = \Gamma_L\Gamma_R/4$ after simple calculation. It is in fact the perfect transmission condition in the case of double sites. Physically the even-odd dependence of conductance reflects the different conditions of constructive interference in the different circumstances. For the lattice with odd number of sites, one can view the array as a single site coupled with two renormalized leads. If the number of sites is even, the lattice can be considered as a two renormalized normal metal contact or a double sites coupled with two renormalized leads. The condition for perfect transmission is more strict in the later case.

Finally, we would like to discuss possible effects arising from electron-electron interaction. It is expected that the main results may hold as well. In the presence of on-site Coulomb interaction, an additional term of self-energy will be introduced for the Green function of each site. The effect is just shifting the site level and splitting the resonance position at absolute
zero temperature, since elastic scattering can only be expected at zero temperature.\textsuperscript{30} The central formula (23) remains formally the same in the presence of interactions as long as the ground-state of the system possess Fermi liquid properties.\textsuperscript{31}

IV. CONCLUSIONS

In summary, using the Keldysh nonequilibrium Green function method, we have derived the formulas to calculate the transmission coefficient, current and conductance of a chain of coupled $N$ site system. An effective and convenient procedure to calculate recursively the retarded(advanced) and lesser(greater) Green functions has been developed. Based on the formulation developed, we have analyzed the transmission spectra of just single site, double site and triple site structures in detail, obtaining some well-know results and finding some new features in the transmission spectra of double and triple site systems. When the electron levels of $N$ sites are aligned, we have obtained an analytical expression for the condition for perfect transmission, demonstrating the even-odd parity effect in the transmission of a generic one dimensional lattices with inversion symmetry.

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FIG. 1: Transmission spectra of a double site structure in the case of symmetric (a,c) and asymmetric (b,d) site-lead couplings.

FIG. 2: Transmission spectra of a triple site structure in the case of symmetric site-lead couplings ($\Gamma_L = \Gamma_R = 1$): (a)$\epsilon_1 = \epsilon_2 = \epsilon_3 = 10$; (b)$\epsilon_1 = 9, \epsilon_2 = 10, \epsilon_3 = 11$; (c)$\epsilon_1 = 9, \epsilon_2 = 11, \epsilon_3 = 9$ and (d)$\epsilon_1 = 9, \epsilon_2 = 9, \epsilon_3 = 11$.

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FIG. 3: Transmission spectra of a triple site structure in the case of asymmetric site-lead couplings ($\Gamma_L = 1, \Gamma_R = 4$): (a)$\epsilon_1 = \epsilon_2 = \epsilon_3 = 10$; (b)$\epsilon_1 = 9, \epsilon_2 = 10, \epsilon_3 = 11$; (c)$\epsilon_1 = 9, \epsilon_2 = 11, \epsilon_3 = 9$ and (d)$\epsilon_1 = 9, \epsilon_2 = 9, \epsilon_3 = 11$. 
fig.1 zeng et al.
fig.2 zeng et al.

(a) $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 10$
- $t_L = t_R = 0.3$
- $t_L = t_R = 1$
- $t_L = t_R = 2$
- $\Lambda_L = \Lambda_R = 0.1$
- $t_L = 1$, $t_R = 4$

(b) $\varepsilon_1 = 9$, $\varepsilon_2 = 10$, $\varepsilon_3 = 11$
- $t_L = t_R = 0.5$
- $t_L = t_R = 2$
- $t_L = 1$, $t_R = 4$
- $t_L = 4$, $t_R = 1$

(c) $\varepsilon_1 = \varepsilon_3 = 9$, $\varepsilon_2 = 11$
- $t_L = t_R = 0.5$
- $t_L = t_R = 2$
- $t_L = 1$, $t_R = 4$

(d) $\varepsilon_1 = \varepsilon_2 = 9$, $\varepsilon_3 = 11$
- $t_L = t_R = 0.5$
- $t_L = t_R = 2$
- $t_L = 1$, $t_R = 4$
- $t_L = 4$, $t_R = 1$

Transmission vs. $\varepsilon$ (arb. units)
fig. 3 Zeng et al.