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Transmittance anomalies of a ring with lead-positional asymmetry

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Abstract. We examine the anomalous behavior of the transmittance through a one-dimensional ring having two branches of different lengths, as determined by the lead positions. Jumps in the transmittance phase are occurring in correspondence to both (a) zeros in the transmission at the eigenstates of the isolated ring and (b) destructive interference events. It is also found that when the ratio of the branch lengths is given by p/q satisfying $p + q = 0 \pmod 4$, the two characteristic zeros merge into a single point and the transmittance phase becomes identical to the so-called Friedel phase.

PACS. 03.65.Bz Foundations, theory of measurement, miscellaneous theories (including Aharonov-Bohm effect, Bell inequalities, Berry's phase) – 11.30.Er Charge conjugation, parity, time reversal, and other discrete symmetries – 03.65.-w Quantum mechanics – 05.60.-k Transport processes

Introduction

Recent experiments by Yacoby *et al.* [1] and by Schuster *et al.* [2] have attracted much interest into phase-sensitive transport. In these measurements, when sweeping the gate voltage, the relative phase between incoming and outgoing waves traversing a quantum dot was found to increase smoothly by π while crossing the transmission resonances (the latter being well described by the Breit-Wigner formula [3]). Additionally, the zeros in the transmission are also accompanied by an even more intriguing phase feature, as the phase *abruptly* changes by π [2]. Several theoretical studies [4–6] have been successful in describing the observed effects.

When studying the transmittance properties for various scatterers, reflection- and time-reversal-symmetry have been intensively discussed, but less attention has been paid to the influence of the lead positions on the transmittance. This paper intends to explore a ring structure having two branches of *different* lengths (see Fig. 1) determined by the lead positions. Such a system, providing distinct transmission zeros and an interesting associated phase behavior, is already a theoretically interesting fundamental problem by its own. Nevertheless, recent electron transport experiments suggest that the application of these ideas is already in sight. By making use of scanning tunnelling microscope (STM) tips enhanced by the attachment of fragments of carbon nanotubes (CNTs), Watanabe *et al.* [7] have managed to contact a CNT ring to two CNT-STM tips. Their measurements clearly show the possibility of scanning the surface of the ring in a wide range of configurations other than the symmetric probing.

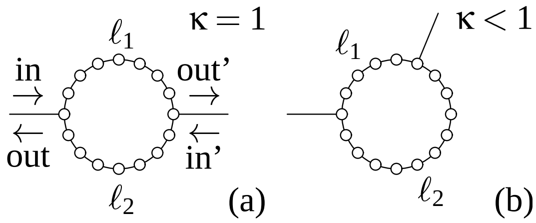

Fig. 1. A schematic view of a ring of $N = 16$ sites, with the same branch lengths (a) and with different lengths (b). Different configurations are classified by the length ratio $\kappa = \ell_1/\ell_2$. Note that κ and κ^{-1} correspond to equivalent configurations.

General definitions

In order to concentrate on the basic physical features that the ring topology offers, we investigate here the transport properties of a one-dimensional ring by means of the scattering matrix $\mathbf{S}$ relating the incoming and outgoing states

$$\begin{pmatrix} \text{out} \\ \text{out'} \end{pmatrix} = \mathbf{S} \begin{pmatrix} \text{in} \\ \text{in'} \end{pmatrix}, \tag{1}$$

with

$$\mathbf{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \mathrm{e}^{\mathrm{i}\vartheta} \begin{pmatrix} \mathrm{i}\mathrm{e}^{\mathrm{i}\varphi_1} \sin\phi & \mathrm{e}^{\mathrm{i}\varphi_2} \cos\phi \\ \mathrm{e}^{-\mathrm{i}\varphi_2} \cos\phi & \mathrm{i}\mathrm{e}^{-\mathrm{i}\varphi_1} \sin\phi \end{pmatrix}. \tag{2}$$

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Let us simplify the situation by considering a system with time-reversal and reflection-symmetry, *i.e.*, $t = t'$ and $r = r'$, leading to $\varphi_{1,2} = 0$ [8]. The remaining quantities, ϑ and ϕ, depend on the incident particle energy as well as the scatterer states, however we omit this dependence for notational simplicity. The transmittance coefficient can be expressed by its modulus and phase as $t = |t|e^{i\vartheta_t}$. If the corresponding transmission, $|t|^2$, is non-zero, ϑ_t must be a continuous function of the energy and is equivalent to ϑ up to an additive constant (which we assume to be zero in what follows). However, when the system undergoes a transmission zero in association with a sign change of $\cos\phi$, the transmittance phase ϑ_t exhibits a discontinuity (a π jump), implying the relation

$$\vartheta_t = \vartheta + \pi\Theta(-\cos\phi), \tag{3}$$

with Θ being the Heaviside function ($\Theta(x) = 1$ if $x > 0$ and $\Theta(x) = 0$ otherwise). Another phase of importance in scattering problems is the so-called Friedel phase [9],

$$\vartheta_{\mathrm{F}} = \frac{1}{2\mathrm{i}} \ln \det \mathbf{S} = \vartheta + \frac{\pi}{2}\cdot \tag{4}$$

While ϑ and ϑ_F are not directly observable, the transmittance phase ϑ_t is the one being detected in experiments. Its behavior, dependent on the lead configuration, is our main concern throughout this paper.

Asymmetric lead configuration

So far, the above mentioned effects have been considered only for symmetric lead configurations, as shown in Figure 1a. Here, we are concerned with the general situation in which the leads contact a one-dimensional ring at different, not necessarily antipodal positions, see Figure 1b. As shown below, by breaking the positional lead symmetry in this way, our system may display zeros in the transmission being forbidden in the symmetric case; in correspondence to these zeros, the transmittance phase undergoes π jumps. Moreover, under the effect of a particular symmetry (see below), two neighboring zeros in the transmission can get closer and closer, and eventually coincide. In such a case, two π jumps can occur at a single point and cancel each other, leaving the transmittance phase effectively unchanged [11]. Another situation in a system with asymmetric probing might arise when a π jump does not occur due to the sign change in $\cos\phi$, but simply due to a discontinuity in ϑ.

System

Our system is an N site ring, eventually considered in the mesoscopic limit $1 \ll N < \infty$, as shown in Figure 1. We can write down the ring Hamiltonian as $(\mathbf{H}_{\mathrm{ring}})_{ij} = \varepsilon_0\delta_{ij} - \gamma(\delta_{ij+1} + \delta_{ij-1})$ with ε_0 and γ being the uniform site energy and hopping strength, respectively. The eigenenergies can be obtained by the secular equation $\det[\varepsilon\mathbf{I} - \mathbf{H}_{\mathrm{ring}}] = 0$, yielding $\varepsilon_n = \varepsilon_0 - 2\gamma\cos(2\pi n/N)$ with $n = 1, \ldots, N$. For convenience, without loss of generality, we set the lattice constant to unity, and we consider even values of N to allow for an antipodal lead configuration. We also fix the position of one of the two leads to 1, whereas the second lead is connected at j, the latter being restricted to $2 \le j \le N/2$. The retarded Green function of the problem, $\mathbf{G} = [(E+\mathrm{i}0^+)\mathbf{I} - \mathbf{H}_{\mathrm{ring}} - \mathbf{\Sigma}]^{-1}$, is given by the isolated ring Hamiltonian, $\mathbf{H}_{\mathrm{ring}}$, and by the self-energy due to the coupling to the external leads, $\mathbf{\Sigma}$, assumed to be energy independent (wide-band limit) [12]. According to the Fisher-Lee relation [13], the connection of the retarded Green functions to the transmittance coefficient reads as $t = -2\mathrm{i}\Gamma\mathbf{G}_{1j}$ where we have assumed equal leads $\Sigma = \mathbf{\Sigma}_{11} = \mathbf{\Sigma}_{jj}$ and $\Gamma \equiv -\mathrm{Im}(\Sigma)$. In order to evaluate the transmittance, we need to calculate the bare Green function $\mathbf{G}_{(\mathbf{\Sigma}=\mathbf{0})}$, and thus its cofactor $\mathcal{C}$ at the lead positions. The Green function entering the transmittance formula hence reads

$$\mathbf{G}_{1j} = \frac{\mathcal{C}_{1j}}{\det\mathbf{Q}} \det\mathbf{G}^{-1}_{(\mathbf{\Sigma}=\mathbf{0})} \tag{5}$$

with

$$\mathbf{Q} = \begin{pmatrix} \det\mathbf{G}^{-1}_{(\mathbf{\Sigma}=\mathbf{0})} - \Sigma\mathcal{C}_{11} & -\Sigma\mathcal{C}_{1j} \\ -\Sigma\mathcal{C}_{j1} & \det\mathbf{G}^{-1}_{(\mathbf{\Sigma}=\mathbf{0})} - \Sigma\mathcal{C}_{jj} \end{pmatrix}\cdot \tag{6}$$

It is worthwhile to note that the above expression applies to any system with atomic contacted leads. Using the system Hamiltonian $\mathbf{H}_{\mathrm{ring}}$, we can obtain the cofactor

$$\mathcal{C}_{1j} = \gamma^{j-1}\mathcal{T}_{N-j} + (-1)^{N-2}\gamma^{N-j+1}\mathcal{T}_{j-2}. \tag{7}$$

Here, $\mathcal{T}_m$ is the determinant of the $m \times m$ tridiagonal matrix whose diagonal and outer diagonals are $E - \varepsilon_0$ and γ, respectively, and is given by $\mathcal{T}_m = (\eta_+^{m+1} - \eta_-^{m+1})/(\eta_+ - \eta_-)$ with $\eta_\pm \equiv (E-\varepsilon_0) \pm \sqrt{(E-\varepsilon_0)^2 - 4\gamma^2}$. Additionally, one can get that $\eta_\pm \equiv \gamma e^{\pm ik}$, where $\tan^2 k \equiv 4\gamma^2/(E - \varepsilon_0)^2 - 1$. Let us now define the two branch lengths as $\ell_1 = j-1$ and $\ell_2 = N-(j-1)$, so that $\ell_1 \le \ell_2$. The ratio of these two lengths is then expressible as $\kappa = \ell_1/\ell_2 = p/q$ with $p \le q$ being coprime integers. Note that there is a duality symmetry when $\kappa \leftrightarrow \kappa^{-1}$. The two integers define the symmetry order $n \equiv p+q$ for the device configuration, as it necessitates an n-time rotation by an angle $2\pi/(\kappa^{-1}+1)$ to recover the original position of the leads.

After some algebra, we obtain a compact form for the cofactor,

$$\mathcal{C}_{1j} \propto \sin(\pi\beta/2)\cos(\pi\alpha/2). \tag{8}$$

The suitable normalizations of the momentum $\alpha \equiv k(\ell_1 - \ell_2)/\pi$ and $\beta \equiv k(\ell_1 + \ell_2)/\pi$ serve in measuring the commensurability of the wavelength with the length difference between the two branches and the circumference of the ring, respectively. It can be easily noticed that the transmission reaches its zeros either for even-integer β's or for odd-integer α's. The former corresponds to the condition for eigenstates of the isolated ring given by $\det\mathbf{G}^{-1}_{(\mathbf{\Sigma}=\mathbf{0})} = \gamma^N[\cos(\pi\beta) - 1] = 0$, while the latter occurs at points of destructive interference at the nodes. It

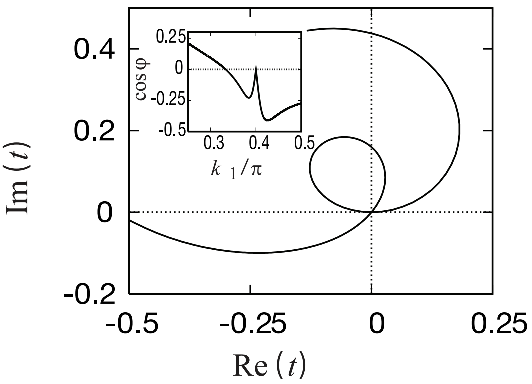

Fig. 2. Transmittance t in the complex plane for $\kappa = 1/4$, evaluated in the momentum interval $k\ell_1 \in [\pi/5, \pi/2]$ in which there exist two single zeros caused by an eigenstate at $k\ell_1 = 2\pi/5$ and by destructive interference at $k\ell_1 = \pi/3$. The inset shows the behavior of $\cos\phi$ a function of $k\ell_1/\pi$.

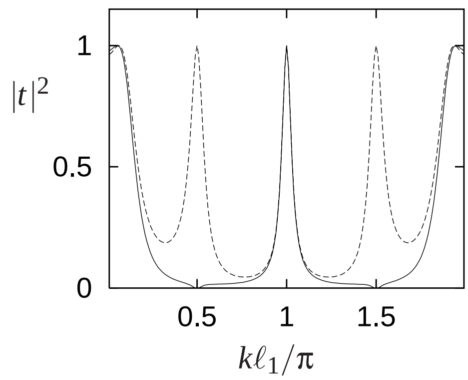

Fig. 3. Transmission $|t|^2$ as a function of momentum $k\ell_1/\pi$. The solid line represents the case $\kappa = 1/3$, and the dashed line shows the symmetric case $\kappa = 1$ for comparison.

is important to note that in the symmetric configuration $\ell_1 = \ell_2$ ($\alpha = 0$), transmission zeros due to destructive interference cannot occur. Furthermore, those zeros in correspondence of the isolated ring eigenstates can neither be achieved in the case $\kappa = 1$, as it will be discussed in the next section. It should also be stressed that the factorization in equation (8) is a general feature of the ring topology and does not depend on the particular choice of lead self-energy studied here. The choice of the latter is motivated by the wish to avoid spurious effects due to the leads which might mask topology induced features [12].

Zeros in the transmission

First, we examine the characteristic zeros in the transmission associated with the eigenstates of the isolated ring which are a sufficient condition for the phase jumps. To this end, in order to show the absence of zeros in the symmetric case, we explicitely write down the determinant of $\mathbf{Q}$ for $\kappa = 1$,

$$\det \mathbf{Q}|_{\kappa=1} = A(\Sigma, \beta) \det \mathbf{G}^{-1}_{(\mathbf{\Sigma=0})} \sin(\pi\beta/2), \tag{9}$$

with the prefactor $A(\Sigma, \beta)$ not vanishing for the eigenstates. Hence, the term $\det \mathbf{G}^{-1}_{(\mathbf{\Sigma=0})} \sin(\pi\beta/2)$ cancels the numerator in equation (5) (after inserting Eq. (8)) and does not yield any zero in the transmission. On the contrary, when $\kappa < 1$ and when the eigenstates condition (even-integer β's) and the constructive interference one (even-integer α's) are not simultaneously satisfied, such cancellation does not occur, causing zeros in the transmission at the eigenstates. Furthermore, in the case $\kappa < 1$, the phase difference can lead to destructive interference at the lead positions, also resulting in zeros in the transmission.

Transmittance phase: Single zeros

We examine now the transmittance phase at the single zeros in the transmission, located at certain $k\ell_1$ in accordance with either eigenstates or destructive interference. As an example, we choose the length ratio as $\kappa = 1/4$, for which an eigenstate occurs at $k\ell_1 = 2\pi/(4+1)$, whereas $k\ell_1 = \pi/(4-1)$ leads to destructive interference. For this purpose, it is helpful to have a look at the transmittance in the complex plane, which is presented in Figure 2 for the momentum regime of $k\ell_1 \in [\pi/5, \pi/2]$. (It should be noted that $k\ell_1$ can be changed by either changing the energy E or the position j of the second lead.) The trajectory starts from the third quadrant and ends in the second quadrant. Across the first zero occurring at $k\ell_1 = \pi/3$, the trajectory is traced from the third to the first quadrant, yielding a sign change both in real and in imaginary part of the transmittance. On the other hand, for the second zero at the eigenstate $k\ell_1 = 2\pi/5$, the trajectory passes through the origin from the second to the first quadrant, and thus the sign change only occurs in the real part of the transmittance. In both cases, when passing through the single zero in the transmittance, a π jump in ϑ_t occurs (see Fig. 2). Decomposing the transmittance into real and imaginary part as $\mathrm{Re}(t) = \cos\vartheta \cos\phi$ and $\mathrm{Im}(t) = \sin\vartheta \cos\phi$, we notice that the π jump achieved by destructive interference is due to the sign change of the common factor $\cos\phi$. However, this is not the case for the π jump due to the eigenstate. As the inset in Figure 2 shows, the sign change in $\cos\phi$ occurs only across the transmission zero due to the destructive interference, not at the zero due to the eigenstate. This is also confirmed by the evaluation of transmittance to reflectance ratio, $t/r = \cot\phi$, where the reflectance is determined in terms of the Green function as $r = 1 - 2\mathrm{i}\Gamma \mathbf{G}_{11}$. It indicates that the π jump in ϑ_t at the transmission zero due to the eigenstate is accompanied by a π jump in ϑ.

Transmittance phase: Double zeros

Finally, we examine the cases in which the system symmetry allows two characteristic zeros to coincide. In Figure 3, we present the transmission for $\kappa = 1/3$ as solid line, and that for the symmetric case $\kappa = 1$ as dashed line, in which

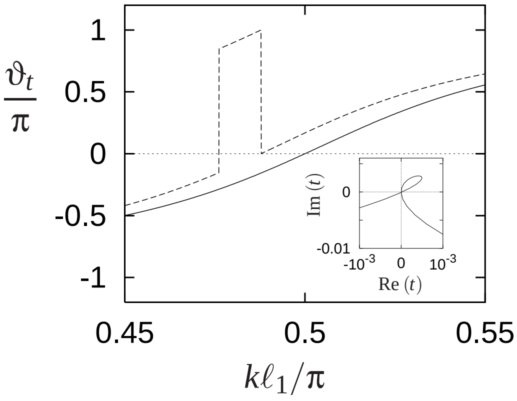

Fig. 4. Transmittance phase ϑ_t/π *versus* momentum $k\ell_1/\pi$, shown for $\kappa = 1/3$ as solid line. The transmittance phase exhibits no jump, even across the (double) zero in the transmission occurring at $k\ell_1 = \pi/2$. For comparison, the transmittance phase for $\kappa = 10/31$ is presented as dashed line (in both cases, $\epsilon = 10^{-7}$ is used). The inset shows the transmittance coefficient in a complex plane near the zero in the transmission for $\kappa = 10/31$.

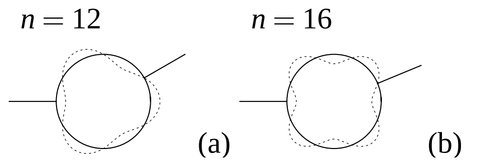

Fig. 5. Schematic configurations for the occurrence of double zeros in the transmission for different symmetry orders (a) $n = 12$ and (b) $n = 16$. To identify the Friedel phase with the transmittance phase, the outgoing leads can be located at any nodal points given by the crossings between the ring and the standing waves, the latter drawn as dashed lines.

the resonance lines at $k\ell_1 = n\pi$ are persistent for the asymmetric probing. It is of interest to notice that the zeros at $k\ell_1 = (2n+1)\pi/2$ correspond to the condition for destructive interference as well as for the eigenstates, *i.e.*, for double degenerated zeros in the transmission.

We now investigate what happens to the transmittance phase at the double zeros, for the case $\kappa = 1/3$, in comparison to a case of higher-order symmetry, for example $\kappa = 10/31$. The latter case results in two nearby zeros in the transmission at $k\ell_1/\pi = 10/21$ and $k\ell_1/\pi = 20/41$. Figure 4 displays, as solid line, the transmittance phase for the case $\kappa = 1/3$, and, as dashed line, that for the case $\kappa = 10/31$. For the latter case, the evolution of the transmittance coefficient in the complex plane is shown in the inset of Figure 4. Imagining the radius of the closed loop shrinking as the two characteristic zeros merge into a single point, makes it easy to infer that the transmittance for $\kappa = 1/3$ displays a cusp-like profile. This singular behavior of the transmission can be traced out by introducing $\tilde{k} = k + \mathrm{i}\epsilon$ with a small ϵ. We evaluate the transmittance phase with $\epsilon = 10^{-7}$; Figure 4 displays the continuous evolution of the transmittance phase across the double zero ($k\ell_1 = \pi/2$). As noted already, at the double zero there is no sign change of $\cos\phi$, and therefore, we can identify the transmittance phase with the Friedel phase (up to an additive constant). The general condition for this identity to occur is that $k\ell_1$ is simultaneously an odd-integer multiple of $\pi/(\kappa^{-1} - 1)$ and an even-integer multiple of $\pi/(\kappa^{-1} + 1)$, so that the corresponding symmetry order is characterized by $n = p + q = 0$ (mod 4). In Figure 5, we present two corresponding examples of configurations appropriate for the observation of double zeros.

Conclusions

In summary, we have considered a one-dimensional ring with two external leads attached, where the two branch lengths ℓ_1 and ℓ_2 differ. With the length ratio defined as $\kappa = \ell_1/\ell_2 = p/q$, the configurations of the ring exhibiting smooth behavior of the transmittance phase, ϑ_t, together with double zeros in transmission are found to have the symmetry order $n = p + q = 0$ (mod 4). Furthermore, we have pointed out two causes leading to π jumps in ϑ_t, one of which being simply due to the destructive interference at the external lead positions and followed by overall sign change in t across the zeros. The other one, even more interesting, is that *asymmetric* lead-positions allow to probe eigenstates revealed by zeros in the transmission. This is in contrast to the case of symmetric leads where the eigenstates of the isolated system lead to a maximal transmission.

Although the transmittance properties have been already discussed quite generally for various kinds of scatterers [6], the main attention has been paid to the time-reversal- and reflection-symmetry [5]. However, less attention has been paid to the effects due to configurational symmetry of the lead which we have focused on. The effects revealed here are quite striking and are not observable in the traditional symmetric setup $\kappa = 1$. A word of caution should be spend since our analysis is based on linear chains and not on realistic quasi-onedimensional systems such as carbon nanotubes (CNT). However, numerical calculations for a CNT-ring contacted by CNT leads [14] indicate that the typical scenario depicted here is still valid in a single-electron picture, although many features become much more complex due to spurious effects of the (energy dependent) leads. Therefore, we believe that our predictions might probably be observable in pure carbon set-up [7]. Finally, we think that our findings, besides being of theoretical interest from a fundamental point of view, might also open some interesting directions to applicative purposes.

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12. The choice of wide-band leads is justified by the fact that more realistic choices such as semi-infinite CNTs, although significantly increasing the complexity of both the treatment and the results, do not alter the basic features discussed in this work [14]. In particular, keeping the treatment on the present level allows for a full investigation of the behavior of the phase at the transmission singular points
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