Transport Fano filter

J. Klier,1 I.V. Krainov,2,3 A.P. Dmitriev,2 and I.V. Gornyi1,2

1Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany
2Ioffe Physico-Technical Institute of the Russian Academy of Sciences, 194021 St. Petersburg, Russia
3Lappeenranta University of Technology, P.O. Box 20, FI-53851, Lappeenranta, Finland

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We show that the presence of a side-attached state strongly modifies the transmission through a one-dimensional double-barrier system in the window of wavevectors around the Fano antiresonance. Specifically, the interplay between the Fano interference and the size quantization inside the structure gives rise to a narrow resonant peak in the transmission coefficient. The height of the peak may become close to unity (perfect transmission) even for an asymmetric setup with strong barriers, where the transmission coefficient is strongly suppressed at all other wavevectors. Thus, the structure can be used as a filter of monochromatic waves in nanoelectronic and photonic devices.

I. INTRODUCTION

Fano resonant suppression [1] of the wave transmission in the presence of a localized discrete state is one of the most famous interference phenomena in atomic physics, optics, and electronics (for reviews, see Refs. [2, 3]). It is well known that the amplitude $A$ of the electron transition to the states of a continuum through a localized quasistationary level $\varepsilon_0$ is described by the Breit-Wigner formula

$$A = i A_0 \frac{\Gamma}{\varepsilon - \varepsilon_0 + i\Gamma},$$

(1)

where $\varepsilon$ is electron’s energy, $\Gamma$ is the width of the level, and the magnitude $A_0$ does not vary with energy on the scale of the order of $\Gamma$. The probability of transition demonstrates the symmetrical resonance of the usual Lorentz form. If, in addition to the resonant transition through the intermediate level, a direct transition with an amplitude $B$ that weakly depends on energy is also allowed, the total transition amplitude is equal to the sum of the amplitudes $A$ and $B$. Then an interference term $2\text{Re}(AB^*)$ appears in the expression for the transition probability

$$W = |A + B|^2 = |B|^2 \frac{(|\varepsilon - \varepsilon_0 + i\Gamma(A_0/B + 1)|)^2}{(\varepsilon - \varepsilon_0)^2 + \Gamma^2},$$

(2)

which leads to an asymmetric resonance, first described by Fano [1] for the case of photoionization of the atom. When $A_0/B + 1 = iq$ is purely imaginary, the asymmetry of the Fano resonance is governed by $q$,

$$W = |B|^2 \frac{(|\varepsilon - \varepsilon_0 - q\Gamma)|^2}{(\varepsilon - \varepsilon_0)^2 + \Gamma^2},$$

(3)

which interpolates between the Breit-Wigner resonance for large $q$ and the symmetric Fano antiresonance at $q = 0$. In the latter case, the transition probability is strictly zero at $\varepsilon = \varepsilon_0$.

Since then, a wide variety of physical systems, from mechanical to nuclear, have been studied experimentally and theoretically, in which one of the two interfering amplitudes for transitions into the continuum is resonant. In particular, such a situation is realized for electrons passing through a one-dimensional (1D) system, next to which a tunnel-coupled “atom” is located [2, 4]. An electron trapped on the atom’s level has the energy $\varepsilon_0$ and the lifetime $\hbar/\Gamma$ corresponding to the tunneling coupling between the atom and the wire. The transmission coefficient is then proportional to the ratio $(\varepsilon - \varepsilon_0)^2/[(\varepsilon - \varepsilon_0)^2 + \Gamma^2]$, which corresponds to $q = 0$ in Eq. (3). This means that at $\varepsilon = \varepsilon_0$, the wave corresponding to the capture of an electron on the atom completely “extinguishes” the directly transmitted wave, so that there is full reflection (Fano antiresonance in transmission).

Physics related to the Fano antiresonance is relevant, for example, to complex quantum-dot structures [5], such as a tunnel-coupled carbon nanotubes (CNT) with side-attached single-molecule magnets [6, 7]. These structures received much attention because of the giant magnetoresistance which is caused by a spin-dependent scattering of the conducting electrons on the localized state of a single-molecule magnet [6, 7]. The calculations in the present paper are motivated by our recent work [9] that proposed an explanation of the giant magnetoresistance observed in the Coulomb blockade regime in CNTs with with organic molecules attached to them. The molecules create a quasistationary discrete level for electrons of the CNT, leading to the Fano resonance in the transmission coefficient. In Ref. [9], in accordance with the conditions of the experiments, a rather fast phase breaking was assumed, so that the electron motion between two tunnel barriers was not quantized (the Fano state on the molecule is tunnel-coupled to the continuous spectrum in the CNT). However, of independent interest is the problem of the effect of level quantization on the Fano antiresonance in a coherent quantum dot. This paper is dedicated to solving this problem.

In a 1D system with two strong barriers without a resonant impurity, the transmission coefficient as a function of the electron energy is a “comb” of narrow peaks centered at energies that coincide with the energies of the size quantization levels. We show that the presence of a side-attached state strongly modifies the trans-
mission through a double-barrier system in the window of wavevectors around the Fano antiresonance. Specifically, the interplay between the Fano interference and the size quantization inside the structure gives rise to a narrow resonant peak in the transmission coefficient. Remarkably, the height of the peak may become close to unity (perfect transmission) even for an asymmetric setup with strong barriers, where the transmission coefficient is strongly suppressed at all other wavevectors. The height of this peak, depending on the position of the impurity in the structure, oscillates with an amplitude of the order of its magnitude and a period of the order of the electron wavelength. Thus, the structure can be used as a narrow-band filter in nanoelectronic and photonic devices.

The paper consists of the introduction, three main sections, and the conclusion. In Sec. [I], we recapitulate the basics of the two main ingredients of our analysis separately and introduce the notations. First, the transmission of electrons through a 1D system with Fano resonance and without tunneling barriers is addressed in Sec. [IIA]. Next, a double-barrier system is considered in Sec. [IIB]. In Sec. [III], the problem of the transmission of an electron through a 1D system with two tunnel barriers and Fano resonance between them is solved. In Sec. [IV], the emergent narrow transmission resonance is analyzed.

II. BASICS

A. Transmission across a Fano state

We start with the analysis of the influence of a Fano state on transport in an infinite one-dimensional (1D) channel. Throughout the paper, we consider a single-particle problem. In the presence of electron-electron or electron-phonon interactions in a single-channel wire, the wire conductance in the presence of a side-attached localized state have been studied in Refs. [10, 11] and [12]. The Hamiltonian of 1D free electrons which can tunnel to a side-attached localized state reads:

\[ \hat{H} = \sum_k E_k |\psi_k\rangle \langle \psi_k| + \sum_k (\varepsilon_0 |\varphi\rangle \langle \varphi| + V_k |\psi_k\rangle \langle \psi_k| + V_k^* |\varphi\rangle \langle \varphi|). \]

(4)

Here, \( \varepsilon_0 \) denotes the energy of the localized state with the corresponding wave function \( \varphi \), \( E_k = \hbar^2 k^2/(2m) \) and \( \psi_k \) are the energy and wave function of state \( k \) in the 1D channel, \( V_k = \langle \varphi|\hat{V}|\psi_k\rangle \) is the Bardeen tunneling matrix element \([13]\) of the tunneling operator \( \hat{V} \). The wave functions \( \varphi \) and \( \psi_k \) are assumed to be orthogonal to each other.

The transmission \( (t_F) \) and reflection \( (r_F) \) amplitudes for the localized Fano state are given by [2]:

\[ t_F = \frac{E_k - \varepsilon_0(k)}{E_k - \varepsilon_0(k) + i\Gamma_0(k)}, \]

(5)

\[ r_F = \frac{-i\varepsilon_0(k)}{E_k - \varepsilon_0(k) + i\Gamma_0(k)}, \]

(6)

where (the dash denotes the principal-value integral)

\[ \varepsilon_0(k) = \varepsilon_0 + \int_0^\infty dp \frac{|V_p|^2}{E_k - E_p}, \]

(7)

\[ \Gamma_0(k) = \pi \int_0^\infty dp \delta(E_p - E_k)|V_p|^2. \]

(8)

For a pointlike tunneling, \( V_p \) is momentum independent, and hence there is no \( k \) dependent shift of the Fano-state energy and the suppression of the transmission is symmetric. In the general case, we introduce \( k_0 = \sqrt{2m\varepsilon_0/\hbar^2} \) and \( \Gamma_0 = \Gamma_0(k_0) \) (for weak tunneling, it is sufficient to take \( \varepsilon_0(k) \) and \( \Gamma_0(k) \) at the resonant point). The energy scale \( \Gamma_0 \) describes the broadening of the localized state, which stems from the coupling between the 1D channel and localized state. The Fano state suppresses the transmission in the window of resonant energies \( E_k \sim (\varepsilon_0 - \Gamma_0, \varepsilon_0 + \Gamma_0) \). For a confined geometry, however, the broadening of the Fano resonance is changed by the properties of the boundaries and may also be momentum dependent, as we will discuss in the following sections.

A schematic illustration of the processes responsible for the Fano resonance is presented in Fig. 1. This figure shows the interference of the electronic wave that passes through the wire with the continuous spectrum directly, i.e., without visiting the Fano state, and the wave that passes via scattering on the discrete state (paths 1 and 2 in Fig. 1, respectively). Exactly at the resonance, \( E_k = \varepsilon_0 \), path 2 acquires a phase of \( \pi \) leading to zero transmission, since the sum of the two waves vanishes \( e^{ikx} + e^{ikx+\pi^\ast} = 0 \). Accordingly, the reflection coefficient reaches maximum (unity) at the resonance.
B. Double-barrier structure

In this section, we present a description of a double-barrier structure in the absence of the Fano state. Again, as in Sec. IIIA above, we do not consider here effects of electron-electron interactions in the wire, which would lead to a peculiar renormalization of the transmission coefficient through the structure, see Refs. [14–17].

Without loss of generality, we model the tunnel contacts as two δ-function barriers characterized by strength $\eta_l$ and $\eta_r$ for the left and right barrier, respectively. We introduce the wave-functions for the system with two barriers located at $x = \pm L$ and decompose it into the symmetric and antisymmetric parts as

$$
\Psi_{k+}(x) = \begin{cases} 
\cos(kx) + \frac{\eta_r \cos(kL)}{k} \sin[k(x-L)], & x \geq L, \\
\cos(kx), & |x| \leq L, \\
\cos(kx) - \frac{\eta_l \cos(kL)}{k} \sin[k(x+L)], & x \leq -L,
\end{cases}
$$

and the left moving wave is given by

$$
\Psi_{k-}(x) = \begin{cases} 
\sin(kx) + \frac{\eta_r \sin(kL)}{k} \sin[k(x-L)], & x \geq L, \\
\sin(kx), & |x| \leq L, \\
\sin(kx) + \frac{\eta_l \sin(kL)}{k} \sin[k(x+L)], & x \leq -L,
\end{cases}
$$

The right-moving wave is described by

$$
\phi_{+k}(x) = a_{+l}(k)\Psi_{k+}(x) + a_{-l}(k)\Psi_{k-}(x),
$$

and the left moving wave is given by

$$
\phi_{-k}(x) = a_{+l}(k)\Psi_{k+}(x) - a_{-l}(k)\Psi_{k-}(x).
$$

Here, the coefficients are given by

$$
a_{r+,l+}(k) = \frac{2k}{D(k)} [k + \eta_r \sin(kL) \exp(ikL)],
$$

$$
a_{r-,l-}(k) = \frac{2k}{D(k)} [ik - \eta_r \cos(kL) \exp(ikL)],
$$

with

$$
D(k) = [ik - \eta_l \cos(kL) e^{ikL}] [k + \eta_r \sin(kL) e^{ikL}] + [k + \eta_l \sin(kL) e^{ikL}] [ik - \eta_r \cos(kL) e^{ikL}].
$$

For the case of symmetric setup with $\eta_r = \eta_l = \eta$, we get $a_{r+} = a_{l+} = a_+$ and $a_{r-} = a_{l-} = a_-$, where

$$
a_+(k) = \frac{ik}{ik - \eta \cos(kL) \exp(ikL)},
$$

$$
a_-(k) = \frac{ik}{k + \eta \sin(kL) \exp(ikL)}.
$$

Using these equations, we express the transmission and reflection coefficients of the symmetric double-barrier structure as:

$$
t_{BB}(k) = \frac{1}{2} \left[ \frac{a_+(k)}{a_+^*(k)} - \frac{a_-(k)}{a_-^*(k)} \right],
$$

$$
r_{BB}(k) = \frac{1}{2} \left[ \frac{a_+(k)}{a_+^*(k)} + \frac{a_-(k)}{a_-^*(k)} \right].
$$

These formulas describe resonances at energies corresponding to the size quantization levels. For the symmetric setup, the transmission coefficient $t_{BB}(k) = |t_{BB}|^2$ is equal to unity at resonances at $k = k_n$, where $k_n$ are determined from the equation

$$
tan(2kL) = -\frac{2k}{\eta}.
$$

For strong barriers $\eta \gg k, 1/L$, one finds $k_n \approx (\pi n/2)[1 - (\eta L)^{-1}]$. The transmission coefficient is then described by a standard Breit-Wigner formula.

For an asymmetric setup with $\eta_r \neq \eta_l$, the transmission amplitude can still be written through $D(k)$ from Eq. (15) as

$$
t_{BB}(k) = k/D(k).
$$

The transmission coefficient then also shows resonances (for strong barriers again described by the Breit-Wigner formula), but the height of the resonances is now always smaller than unity.

We will use the notation introduced in this section in Sec. III where a Fano state inside the double-barrier structure is considered.

III. DOUBLE-BARRIER STRUCTURE WITH A FANO STATE

A. Formalism

If the 1D channel hosting the Fano state is tunnel-coupled to external leads, the resonant interference of electron waves scattered of the tunnel barriers becomes...
important. With the Fano state side-attached to the region of the wire inside the double-barrier structure (Fig. 2), the Hamiltonian of the system,

$$\hat{H} = \hat{H}_0 + \varepsilon_0 |\varphi\rangle \langle \varphi|$$
$$+ \int_0^\infty dk \left( V_{-k} \psi_{-k} \langle \varphi| + V_{-k}^* \langle \psi_{-k}| \right)$$
$$+ \int_0^\infty dk \left( V_{+k} \psi_{+k} \langle \varphi| + V_{+k}^* \langle \psi_{+k}| \right). \quad (22)$$

is modified compared to Eq. (4) by accounting for a quasi-discrete spectrum. In Eq. (22), $\hat{H}_0$ is the Hamiltonian of the 1D wire with the two barriers. The corresponding eigenfunctions are given by

$$\psi_{\pm k}(x, r_\perp) = \phi_{\pm k}(x) \xi(r_\perp)$$

with $\phi_{\pm k}(x)$ given by Eqs. (11) and (12). The matrix elements $V_{\pm k}$ of the tunneling operator $V$ are defined with respect to these eigenfunctions. The function $\xi(r_\perp)$ depends on the coordinate transverse to the wire. The energy $\varepsilon_0$ is the energy of the discrete level located at position $x = a$ with the corresponding wave function $\varphi(x, r_\perp)$. The functions $\psi_{\pm k}(x, r_\perp)$ and $\varphi(x, r_\perp)$ are orthogonal to each other because of a zero overlap in the transverse direction.

Let us first analyze the case of symmetric setup with equal barriers characterized by $\eta$. For a symmetric pointlike tunneling operator $V$ and the Fano state located at position $x = a$, the coupling to left and right moving waves is given by

$$V_{+k} = V \left[ a_+|k\rangle \cos(ka) + a_-|k\rangle \sin(ka) \right], \quad (23)$$
$$V_{-k} = V \left[ a_+|k\rangle \cos(ka) - a_-|k\rangle \sin(ka) \right]. \quad (24)$$

Here, $a_+(k)$ and $a_-(k)$ are given by Eqs. (16) and (17) and $V$ is a constant characterizing the strength of tunneling.

The equation for the eigenfunctions $\Phi_{\pm k}$ of the full Hamiltonian, corresponding to electrons moving through the system from left to right, can be written as

$$\Phi_{+k}(x, r_\perp) = \psi_{+k}(x, r_\perp)$$
$$+ \int G_k(x, r_\perp; x', r_\perp') \hat{V} \Phi_{+k}(x', r_\perp') dx' dr_\perp'. \quad (25)$$

Here, $G_k(x, r_\perp; x', r_\perp')$ is the Green's function of the operator $H_0 + \varepsilon_0 |\varphi\rangle \langle \varphi|.

To solve the self-consistent equation for the right moving function Eq. (25), we expand the full function of the system in terms of the eigenfunctions of the Hamiltonian without coupling. With the orthogonality of the functions $\psi_{-k,+k}(x, r_\perp)$ and $\varphi(x, r_\perp)$, we obtain (for brevity, we suppress the arguments $x, r_\perp$ in all eigenfunctions):

$$\Phi_{+k} = \psi_{+k} + \frac{V_{-k}}{E_k - E_0 - \Sigma(k)} \varphi$$
$$+ \frac{V_{+k}}{E_k - \varepsilon_0 - \Sigma(k)} \int_0^\infty dk' \frac{V_{+k'}}{\hat{V} \psi_{+k'} + V_{-k'} \psi_{-k'}} \frac{E_k - E_k' + i0}{E_k - E_k' + i0} \quad (26)$$

with the operator $\hat{V} = V - V_0$ defined by Eqs. (11) and (12). The matrix elements $V_{\pm k}$ of the tunneling operator $V$ are defined with respect to these eigenfunctions. The function $\xi(r_\perp)$ depends on the coordinate transverse to the wire. The energy $\varepsilon_0$ is the energy of the discrete level located at position $x = a$ with the corresponding wave function $\varphi(x, r_\perp)$. The functions $\psi_{\pm k}(x, r_\perp)$ and $\varphi(x, r_\perp)$ are orthogonal to each other because of a zero overlap in the transverse direction.

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The equation for the eigenfunctions $\Phi_{\pm k}$ of the full Hamiltonian, corresponding to electrons moving through the system from left to right, can be written as

$$\Phi_{+k}(x, r_\perp) = \psi_{+k}(x, r_\perp)$$
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Here, $G_k(x, r_\perp; x', r_\perp')$ is the Green's function of the operator $H_0 + \varepsilon_0 |\varphi\rangle \langle \varphi|.

To solve the self-consistent equation for the right moving function Eq. (25), we expand the full function of the system in terms of the eigenfunctions of the Hamiltonian without coupling. With the orthogonality of the functions $\psi_{-k,+k}(x, r_\perp)$ and $\varphi(x, r_\perp)$, we obtain (for brevity, we suppress the arguments $x, r_\perp$ in all eigenfunctions):

$$\Phi_{+k} = \psi_{+k} + \frac{V_{-k}}{E_k - E_0 - \Sigma(k)} \varphi$$
$$+ \frac{V_{+k}}{E_k - \varepsilon_0 - \Sigma(k)} \int_0^\infty dk' \frac{V_{+k'}}{\hat{V} \psi_{+k'} + V_{-k'} \psi_{-k'}} \frac{E_k - E_k' + i0}{E_k - E_k' + i0} \quad (26)$$

with the self-energy

$$\Sigma(k) = \int_0^\infty dk' \left| V_{+k'} \right|^2 + \left| V_{-k'} \right|^2 \frac{E_k - E_k' + i0}{E_k - E_k' + i0}. \quad (27)$$

The real part of the self-energy, which is given by the principal-value integral, determines the position of the shifted resonance, $\varepsilon_0(k) = \varepsilon_0 + \delta\varepsilon_0(k)$, where

$$\delta\varepsilon_0(k) = \int_0^\infty dk' \left| V_{+k'} \right|^2 + \left| V_{-k'} \right|^2 \frac{E_k - E_k' + i0}{E_k - E_k' + i0}. \quad (28)$$

The imaginary part, as usual, describes the broadening of the Fano state,

$$\Gamma(k) = \frac{\pi m}{k} \left( \left| V_{+k} \right|^2 + \left| V_{-k} \right|^2 \right). \quad (29)$$

We are now prepared to calculate the transmission amplitude $t_{\text{BBF}}$ for the Barrier-Fano-Barrier (BFB) structure (Fig. 2), which is done in the following section.

### B. Transmission coefficient

We evaluate the integrals in Eq. (26) at the pole of the denominator, since the other contributions decrease strongly with $x$. The amplitude of the outgoing wave defines the transmission amplitude:

$$t_{\text{BBF}}(k) = \frac{E_k - \varepsilon_0 + (i\pi m/k) \left( \left| V_{-k} \right|^2 - \left| V_{+k} \right|^2 \right)}{E_k - \varepsilon_0 + (i\pi m/k) \left( \left| V_{-k} \right|^2 + \left| V_{+k} \right|^2 \right)} t_{\text{BB}}(k) + \frac{2i(\pi m/k) \left| V_{-k}^* V_{+k} \right|}{E_k - \varepsilon_0 + (i\pi m/k) \left( \left| V_{-k} \right|^2 + \left| V_{+k} \right|^2 \right)} r_{\text{BB}}(k), \quad (30)$$

where $t_{\text{BB}}$ and $r_{\text{BB}}$ are the transmission and reflection coefficients of the double-barrier structure given by Eqs. (18) and (19), respectively.

Using Eqs. (24), we express the combinations of the tunneling matrix elements explicitly through the functions $a_\pm(k)$ from Eqs. (16) and (17). Next, we use the identity following from Eqs. (18) and (19),

$$t_{\text{BB}}(k) = \frac{\text{Re} \left( a_+(k) a_+^*(k) \right) i \text{Im} \left( a_+(k) a_+^*(k) \right)}{i \text{Re} \left( a_+(k) a_+^*(k) \right) \text{Im} \left( a_+(k) a_+^*(k) \right)}.$$
to simplify Eq. (30), leading to \( \Gamma_0 = 2\pi m|V|^2/k \):

\[
t_{\text{BFB}}(k) = \frac{(E_k - \varepsilon'_0)t_{\text{BB}}(k) - i\Gamma_0|a_+|^2 \cos^2(ka) - |a_-|^2 \sin^2(ka)r_{\text{BB}}}{E_k - \varepsilon'_0 + i\Gamma_0|a_+|^2 \cos^2(ka) + |a_-|^2 \sin^2(ka)}. \tag{32}
\]

Expressing the shifted resonance energy as

\[
\varepsilon'_0 = \varepsilon_0 + |V|^2 \int_0^\infty dk' |a_+(k')|^2 \cos^2(k'a) + |a_-(k')|^2 \sin^2(k'a) \frac{dk'}{E_k - E_k'},
\]

we use the following exact relations for the real and imaginary part of the fraction of \(a_+(k)\) and \(a_-(k)\):

\[
\text{Re} \frac{a_+(k)}{a_-(k)} = -i|a_+(k)|^2 \frac{r_{\text{BB}}}{t_{\text{BB}}}, \quad \text{Im} \frac{a_+(k)}{a_-(k)} = -|a_+(k)|^2, \tag{34}
\]

\[
\text{Re} \frac{a_-(k)}{a_+(k)} = -i|a_-(k)|^2 \frac{r_{\text{BB}}}{t_{\text{BB}}}, \quad \text{Im} \frac{a_-(k)}{a_+(k)} = |a_-(k)|^2. \tag{35}
\]

We can now directly evaluate the principal value integral (33) via the Kramers-Kronig relation,

\[
\text{Re} F(x) = \frac{2}{\pi} \int_0^\infty t \text{Im} F(t) \frac{dt}{t^2 - x^2}.	ag{36}
\]

Applying this to Eq. (33) results in

\[
\int_0^\infty dk' \frac{|a_+(k')|^2}{E_k - E_k'} = -\int_0^\infty dk' \frac{k'}{E_k - E_k'} \text{Im} \frac{a_+(k')}{k'a_-(k')},
\]

\[
\text{Re} \frac{a_+(k)}{ka_-(k)} = -\pi m \text{Re} \frac{a_+(k)}{ka_-(k)} = \pi m \frac{i|a_+(k)|^2 r_{\text{BB}}}{t_{\text{BB}}}, \tag{37}
\]

and, similarly,

\[
\int_0^\infty dk' \frac{|a_-(k')|^2}{E_k - E_k'} = -\pi m \frac{|a_-(k)|^2 r_{\text{BB}}}{t_{\text{BB}}}. \tag{38}
\]

The transmission amplitude can then be expressed in a very compact form, reading

\[
t_{\text{BFB}}(k) = \frac{(E_k - \varepsilon_0)t_{\text{BB}}}{E_k - \varepsilon_0 - \Sigma(k)} \tag{39}
\]

with

\[
\Sigma(k) = \Gamma_0 \left[ \frac{a_+(k)}{a_-(k)} \cos^2(ka) - \frac{a_-(k)}{a_+(k)} \sin^2(ka) \right]. \tag{40}
\]

The transmission coefficient \( T_{\text{BFB}} = |t_{\text{BFB}}(k)|^2 \) thus reads:

\[
T_{\text{BFB}}(k) = \frac{T_{\text{BB}} (E_k - \varepsilon_0)^2}{[E_k - \varepsilon_0 + \text{Re}\Sigma(k)]^2 + [\text{Im}\Sigma(k)]^2}. \tag{41}
\]

Note that, somewhat surprisingly, the transmission coefficient \( T_{\text{BFB}} \) is exactly zero at the original energy \( \varepsilon_0 \) of the Fano state, despite the fact that the matrix elements of the tunneling coupling between the localized state and the wire are now momentum dependent. In a continuum spectrum, such a momentum dependence leads to the shift of the energy where the transmission coefficient vanishes, see Eqs. (5) and (7). At the same time, the resonance energy in the denominator is shifted from the value \( \varepsilon_0 \), similarly to Eqs. (5) and (7) for the momentum dependent coupling. This asymmetry between the numerator and denominator in Eq. (41), introduced by the combination of the Fano destructive interference and the level quantization, is a distinct feature of the double-barrier Fano setup.
The hybridization of conducting electrons with the Fano state located at $E_k$ for symmetric barriers and a weak coupling between the Fano state and the wire. The green curve shows the transmission $T_{BFB}$ for the structure with barriers and the Fano state; the black one shows the transmission for two barriers without the molecule $(T_{BB})$. The hybridization of conducting electrons with the Fano state located at $a/L = 0.2$ is characterized by $\Gamma_0 = 1$ meV; the energy of the localized state is $\varepsilon_0 = 5$ meV; the transmission coefficients across the contacts to the leads are the same as in Fig. 3.

The result (41) is illustrated in Figs. 3 and 4. For a strong coupling of the Fano state to the wire, when the Fano-state broadening exceeds the size quantization level spacing, the transmission is suppressed in the region of energies $(E_0 - \Gamma_0, E_0 + \Gamma_0)$, similarly to the case without barriers, Sec. II A. The only difference compared with the continuum case is then in the modulation of the transmission coefficient by the double-barrier resonances, which are now not perfect, in contrast to the case without the Fano state, Sec. II B.

Remarkably, for a weaker coupling of the Fano state, a narrow resonance emerges, Fig. 4 through an interplay of the Fano interference and the size quantization of the spectrum in the double-barrier structure. In the following section, we will analyze this effect in detail.

### IV. EMERGENT RESONANCE

As we see from Fig. 2 for a sufficiently weak coupling between the side-attached Fano state and the wire with quasi-discrete levels, a narrow resonance emerges in the vicinity of the energy of the localized state where the transmission is strictly zero. It is instructive to compare the structure of the obtained transmission coefficient $T_{BFB}$, Eq. (41), with that of the conventional Fano resonance, Eq. (3). Both expressions describe an asymmetric lineshape, with both zero and a maximum present. However, as already emphasized above, $T_{BFB}$ is exactly zero at the original position of the resonant level $\varepsilon_0$. At the same time, at any finite $q$ in Eq. (3), the zero is shifted from $\varepsilon_0$ in the conventional case. Thus, the combined effect of the Fano interference and the size quantization of the spectrum substantially modifies the conventional result (3).

From Eq. (41), we see that the position of the resonance is given by the condition

$$E_k = \varepsilon_0 + \text{Re} \Sigma(k),$$

as in the conventional Breit-Wigner formula, and the width of the resonance is $\text{Im} \Sigma(k)$. Thus, both the position and the width of the resonance depend on momentum. For small $\Gamma_0$, the value of the momentum in $\Sigma(k)$ can be approximated by the momentum corresponding to the of the Fano-state $k_0$. This further implies that the height of the resonance is given by

$$T_{BFB,\text{res}} = T_{BB} \frac{|\text{Re} \Sigma(k)|^2}{|\text{Im} \Sigma(k)|^2} \bigg|_{k=k_0}$$

$$= R_{BB} \left( \frac{|a_+(k)|^2 \cos^2(ka) - |a_-(k)|^2 \sin^2(ka)}{|a_+(k)|^2 \cos^2(ka) + |a_-(k)|^2 \sin^2(ka)} \right)^2 \bigg|_{k=k_0}.$$  

This shows that in the fully symmetric setup, when the Fano state is coupled to the middle of the segment between the barriers, $a = 0$, the height of the peak is given by the reflection coefficient of the double-barrier system:

$$T_{BFB,\text{res}} = R_{BB}, \quad a = 0.$$  

It is clearly seen that for strong barriers, $\eta \gg k$, the transmission coefficient can be very close to unity in the energy window where the transmission through the double-barrier system is suppressed by the destructive interference of waves reflected from the barriers.

The height of the resonant peak for an arbitrary position of the side-attached state can be approximated for
where the general form of $t$ can be again of the order of unity. The expression for the strong resonance with the transmission coefficient that $k_a, L$ ing and width of the emergent resonance oscillate with vary-

Thus, for symmetric strong barriers, the transmission coefficient at the resonance can reach unity (perfect trans-

Importantly, a narrow resonant peak with an almost perfect transmission also emerges for an asymmetric double-barrier setup. In this case, the transmission coefficient $T_{BB}$ for the system without a Fano state is governed by the asymmetry of the structure and can be arbitrarily small. However, the presence of the Fano state leads to a strong resonance with the transmission coefficient that can be again of the order of unity. The expression for the transmission amplitude in this case is given by Eq. (49), where the general form of $t_{BB}(k)$ is given by Eq. (21) and $\Sigma(k)$ reads

in contrast to the tunneling through the localized state, almost perfect transmission through the structure does not re-

Given that the transmission at all other energies is sup-

Before concluding the paper, we would like to mention that it would be interesting to study the emergent reso-

V. CONCLUSION

In this paper, we have shown that the conventional picture of resonant tunneling across a double-barrier struc-

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FIG. 6: Transmission coefficient for the asymmetric double-barrier structure without (green curve) and with a Fano state (black curve) located at $a = 0.63L$ with the level at $k_0 L/2\pi = 5.54$. The barriers are characterized by $\eta_r L/2\pi = 10$, $\eta_l L/2\pi = 100$ and the coupling strength for tunneling between the Fano state and the wire is $\Gamma_0 m L^2/2\pi^2 h^2 = 0.01$.

strong barriers, $\eta \gg k$ (and keeping $|a_+|, |a_-| \ll 1$) as

$$T_{BB, res} = R_{BB} \left[ \frac{\cos(2kL) - \cos(2ka)}{\cos(2kL) \cos(2ka) - 1} \right]^{2}, \quad \text{(45)}$$

defining the momenta where only the antiresonances can appear. The corresponding width of the resonance is given by

$$\text{Im}\Sigma(k_0) = \Gamma_0 \frac{k^2}{\sqrt{2}} \left[ \frac{\cos^2(k_0 a)}{\cos^2(k_0 L) + \sin^2(k_0 L)} \right]. \quad \text{(46)}$$

Thus, for symmetric strong barriers, the transmission coefficient at the resonance can reach unity (perfect trans-

The width of the resonance,

$$\Gamma_{res} \sim \Gamma_0 \sqrt{T_{BB}}, \quad \text{(47)}$$
can be much smaller than the width of the Breit-Wigner peaks in the transmission coefficient $T_{BB}$ for the structure without the side-attached “molecule”. Both the height and width of the emergent resonance oscillate with varying $k, a, L$.

Importantly, a narrow resonant peak with an almost perfect transmission also emerges for an asymmetric double-barrier setup. In this case, the transmission coefficient $T_{BB}$ for the structure without a Fano state is governed by the asymmetry of the structure and can be arbitrarily small. However, the presence of the Fano state leads to a strong resonance with the transmission coefficient that can be again of the order of unity. The expression for the transmission amplitude in this case is given by Eq. (49), where the general form of $t_{BB}(k)$ is given by Eq. (21) and $\Sigma(k)$ reads

$$\Sigma_{asym}(k) = \frac{2\Gamma_0}{a_{r+} a_{r-} + a_{l+} a_{l-}} \left[ a_{r+} a_{l+} \cos^2(ka) - a_{r-} a_{l-} \sin^2(ka) \right] + \frac{a_{l+} a_{r-} - a_{l-} a_{r+}}{2} \cos(ka) \sin(ka), \quad \text{(48)}$$

with $a_{r\pm}$ and $a_{l\pm}$ defined in Eqs. (13) and (14). In the limit of the equal barriers, the result for the self-energy of the symmetric derivation, Eq. (40), is recovered. The emergent resonance for the asymmetric setup is shown in Fig. 6.

Given that the transmission at all other energies is sup-

perfect transmission through the structure does not re-

quire fine-tuning the symmetry of the setup. In addition, the height of the transmission peak can be additionally controlled by changing the location of the side-attached state.

Before concluding the paper, we would like to mention that it would be interesting to study the emergent reso-

nance in the presence of electron-electron and electron-

phonon interactions. For this purpose, an alternative ap-

proach to the calculation of the scattering amplitudes in a double-barrier structure with the Fano state, developed in Ref. [18] on the basis of Green’s function approach, might be useful.
[1] U. Fano, Phys. Rev. 124, 1866 (1961).
[2] A. Miroshnichenko, S. Flach, and Y. Kivshar, Rev. Mod. Phys. 82, 2257 (2010).
[3] Fano Resonances in Optics and Microwaves. Physics and Applications, Springer Series in Optical Sciences, eds. E. Kamenetskii, A. Sadreev, and A. Miroshnichenko (Springer, Berlin 2018).
[4] A.P. Dmitriev, S.A. Emel’yanov, Ya.V. Terent’ev, and I.D. Yaroshetskii, JETP 72, 347 (1991).
[5] W. Gong and C. Jiang, Journal of Applied Physics 106, 013710 (2009).
[6] M. Urdampilleta, S. Klyatskaya, J.-P. Cleuziou, M. Ruben, and W. Wernsdorfer, Nature Materials 10, 502 (2011).
[7] M. Urdampilleta, S. Klyatskaya, M. Ruben, and W. Wernsdorfer, Phys. Rev. B 87, 195412 (2013).
[8] M. Urdampilleta, N.-V. Nguyen, J.-P. Cleuziou, S. Klyatskaya, M. Ruben, and W. Wernsdorfer, International Journal of Molecular Sciences 12, 6656 (2011).
[9] I. V. Krainov, J. Klier, A. P. Dmitriev, S. Klyatskaya, M. Ruben, W. Wernsdorfer, and I. V. Gornyi, ACS Nano 11, 6868 (2017).
[10] I. V. Lerner, V. I. Yudson, and I. V. Yurkevich, Phys. Rev. Lett. 100, 256805 (2008).
[11] M. Goldstein and R. Berkovits, Phys. Rev. Lett. 104, 106403 (2010); Phys. Rev. B 82, 161307 (2010).
[12] A. Galda, I. V. Yurkevich, and I. V. Lerner, EPL 93, 17009 (2011).
[13] J. Bardeen, Phys. Rev. Lett. 6, 57 (1961).
[14] C.L. Kane and M.P.A. Fisher, Phys. Rev. B 46, 7268 (1992).
[15] A. Furusaki and N. Nagaosa, Phys. Rev. B 47, 3827 (1993).
[16] Y.V. Nazarov and L.I. Glazman, Phys. Rev. Lett. 91, 126804 (2003).
[17] D.G. Polyakov and I.V. Gornyi, Phys. Rev. B 68, 035421 (2003).
[18] J. Klier, Magnetotransport in novel Dirac systems, PhD dissertation, Karlsruhe Institute of Technology (published February 2019); DOI: 10.5445/IR/1000090851, https://publikationen.bibliothek.kit.edu/1000090851.