Near-threshold-energy conductance of a thin wire

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We show (1) that a single impurity can have an extremely strong impact on the conductance of a thin wire; (2) that in such a thin wire a couple of two-dimensional impurities may be responsible to strong resonances. (3) Further, we study rough wire transmission in the low-energy regime. We obtain strong localization behavior $T\cong\exp(-L/\xi)$ [L is the wire length and $\xi_{\omega\to\omega_{\rm th}}\sim 1/\ln(\omega-\omega_{\rm th})$, ω is the particle energy and $\omega_{\rm th}\equiv(\hbar\pi/d)^2/2m$ is the threshold energy of a similar wire but without the roughness]. We also show that for very long wires the difference between the threshold energy for transmission ($\omega_{\rm TH}$) and $\omega_{\rm th}$ increases logarithmically with the wire length $\omega_{\rm TH}-\omega_{\rm th}\sim\ln L$. [S0163-1829(99)09639-3]

The passage from one-dimensional (1D) wires to higher dimensional ones is not trivial (see, for example, Refs. 1–4). One-dimensional wires have no width, and thus transversal modes do not exist. The difference between 1D and 2D wires is most pronounced when an incoming wave confronts some sort of imperfection. In this case the scattering picture is not as degenerated as in the 1D case. The wave can be scattered to all directions, while the dynamics become quite complex. A special case is the impact of rough boundaries on conduction (see, for this subject, Refs. 6 and 7). This case is particularly interesting for it is impossible to construct a perfect quantum wire. All the up-to-date techniques (nanolithography, etching and cleaving, epitaxial growth, etc.) reveal their incompetence when dealing with perfect nanostructures. Take, for example, GaAs/AlAs quantum wires grown on a vicinal surface by molecular beam epitaxy.[5] Not only are the boundaries of the GaAs wire quite rough, but there are also impurities of AlAs within it. This is not merely a technological problem, it is clear that any sort of contamination will eventually percolate into the wire (no matter how clean it was initially). Thus, the implications of such imperfections on the conductance are very important.

In this paper we study the transmission through a contaminated wire in the low-energy regime. Within this regime the impurities have their strongest influence on the transmission. Moreover, it is then clear that the higher modes (the first mode is the dominant one) have a negligible contribution, and the wire exhibits a quasi-1D behavior. Thus, we present an exact 2D model of a contaminated wire with the aid of a 2D point scatterer,[8] and investigate it mainly in the low-energy regime.

We first examine the case shown in Fig. 1: A scattering problem over a single surface point defect in a thin wire. The 2D Schrödinger equation is

$$\nabla^2\psi+(E-V)\psi=-D(\mathbf{r}-\mathbf{r}_0)\psi$$

(where we use the units $\hbar=2m=1$). V is the potential of the wire walls ($V=0$ inside the wire and $V=\infty$ outside it), D is the defect potential, and $\mathbf{r}_0=\varepsilon\hat{y}$ is the impurity location. Since the defect has the properties of a pointlike impurity the right-hand term of the Schrödinger equation can be written $D(\mathbf{r}-\mathbf{r}_0)\psi(\mathbf{r}_0)$,[8] which allows for an exact scattering solution.

We hit the impurity with an incoming wave $\psi_{\rm inc}=\sin(\pi y)\exp(i\sqrt{\omega-\pi^2}x)$. In this expression, the length parameters are normalized to the orifice width, i.e., $y=1$ is actually Y (the real coordinate) $=d$ (the orifice width).

Taking advantage of the pointlike nature of the impurity, the scattered wave function due to the defect is[9]

$$\psi_{\rm scar}(\mathbf{r})=\psi_{\rm inc}(\mathbf{r})-\frac{G(\mathbf{r},\mathbf{r}_0)\psi_{\rm inc}(\mathbf{r}_0)}{1+\int d\mathbf{r}'G(\mathbf{r}',\mathbf{r}_0)D(\mathbf{r}'-\mathbf{r}_0)}\int d\mathbf{r}'D(\mathbf{r}'-\mathbf{r}_0), \tag{1}$$

where $G(\mathbf{r}',\mathbf{r}_0)$ is the "outgoing" 2D-Green function of the geometry (the wire). It should be pointed out that if the impurity was not ideal (that is, it was not a point impurity), Eq. (1) would be merely a first-order approximation in the asymptotic solution $|\mathbf{r}|\to\infty$.

The Green function takes the form

$$G(\mathbf{r},\mathbf{r}')\equiv\sum_n\frac{\sin(n\pi y)\sin(n\pi\varepsilon)}{2i\sqrt{E-(n\pi)^2}}e^{i\sqrt{E-(n\pi)^2}|x|}. \tag{2}$$

For the defect potential we choose[8]

$$D(\mathbf{r})\approx d\rho^{-1}\pi^{-1/2}\delta(x)\exp[-y^2/\rho^2], \tag{3}$$

where $\rho\to 0$ is the impurity dimension and d is its strength.

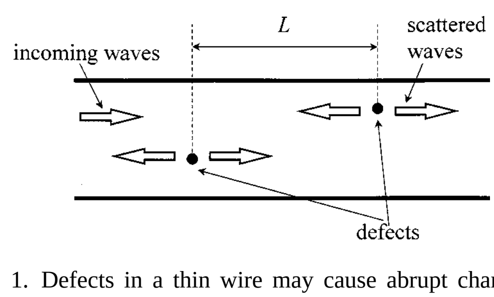

FIG. 1. Defects in a thin wire may cause abrupt changes and resonances in the wire transmission.

Later on, it will be assumed that $\varepsilon \ll 1$ so that the defect is a surface one. Hence,

$$\psi_{sc}(\mathbf{r}) = \psi_{\text{inc}}(\mathbf{r}) + \psi_{\text{inc}}(\mathbf{r}_0) \sum_n a_n \sin(n\pi y) e^{i\sqrt{\psi-(n\pi)^2}|x|}, \tag{4}$$

where

$$a_n \equiv i\frac{\sin(n\pi\varepsilon)}{\sqrt{\omega-(n\pi)^2}} \left[d^{-1} - i\sum_m \frac{\sin^2(m\pi\varepsilon)}{\sqrt{\omega-(m\pi)^2}} e^{-(m\pi\rho/2)^2} \right]^{-1}.$$

Since $\psi_{\text{inc}}(\mathbf{r}_0) = \sin(\pi\varepsilon)$ the scattering coefficient from the first mode to the nth one goes like $t_{1n} \approx n\varepsilon^2$ or generally $t_{kn} \approx kn\varepsilon^2$ (the scattering coefficient from the kth mode to the nth one) and the transmission to the nth mode is thus

$$T \approx (kn)^2 \varepsilon^4, \tag{5}$$

which is an extremely small quantity (since $\varepsilon \ll 1$).

However, when $\omega \approx (m\pi)^2$ for a certain integer m the dynamics could be quite different. When $\omega = (m\pi)^2 + \delta^2$ (for $\delta \ll 1$) the transmitted wave ($x > 0$) becomes

$$\psi_{sc}(\mathbf{r}) \approx \sin(\pi y) e^{i\sqrt{m^2-1}\pi x} \left(1 - \frac{1}{m^2\pi} \frac{\delta}{\sqrt{m^2-1}} \right) - \sin(m\pi y) e^{i\delta x} \frac{1}{m}, \tag{6}$$

that is, the transmission probability from the first mode to the mth mode is

$$T_{1m} \approx \delta/(m^2\pi\sqrt{m^2-1}). \tag{7}$$

Note that the transmission to any other mode is much smaller $T_{1k}(k \neq m) \approx \delta^2$. Equation (7) exhibits no dependence at all on the defect size or strength, any defect will lead to the same result. Surely, Eq. (7) can easily be generalized to any incoming mode $p \neq 1$, and receiving similar dependence, i.e., $T \approx \delta$. However, there is one exception: when the incoming mode is m the dynamics is different.

In this special case, the incoming wave looks like $\psi_{\text{inc}} = \sin(m\pi y)\exp(i\delta x)$, and instead of Eq. (4) we get, $\psi_{sc}(\mathbf{r}) \approx \psi_{\text{inc}}(\mathbf{r}) + \psi_{\text{inc}}(\mathbf{r}_0) a_m \sin(m\pi y)\exp(i\delta|x|)$ where

$$a_m \equiv i\frac{m\pi\varepsilon}{\delta} \left[d^{-1} - i\sum_{m'} \frac{\sin^2(m'\pi\varepsilon)}{\sqrt{\omega-(m'\pi)^2}} e^{-(m'\pi\rho/2)^2} \right]^{-1}. \tag{8}$$

In order to derive Eq. (8) we can use the pointlike character of the defect, i.e., more explicitly $\rho \ll m^{-1}$. Moreover, since we consider a surface defect we have $\varepsilon \ll m^{-1}$ and $\psi_{\text{inc}}(\mathbf{r}_0) = m\pi\varepsilon$.

The summation in Eq. (8) can be rewritten: $\Sigma_{m'} \approx \Sigma_{m'<m} + (m\pi\varepsilon)^2\delta^{-1} e^{-m\pi\rho/2} + \Sigma_{m'>m}$. Each part should be approximated differently to receive (in the limit $\rho \to 0$) $a_m \to im\pi\varepsilon\,\delta^{-1}(d^{-1} - i(m\pi\varepsilon)^2/\delta + \ln(-m\pi\rho/2) + \gamma)^{-1}$ (γ is the Euler's constant). A suitable choice for a 2D scatterer would be an impurity D function (IDF),[8] for which $d^{-1} \equiv \ln(\rho_b/\rho)$. ρ_b characterizes the defect, which is related to its Bohr radius.

The transmitted mode is then $\psi_{sc}(x>0) \approx \sin(m\pi y) e^{i\delta x} t_{mm}$ where the transition coefficient is

$$t_{mm} \approx 1 - \left[1 + i\frac{p\delta}{(m\pi\varepsilon)^2} \right]^{-1}, \tag{9}$$

where $p \equiv \ln(-2\pi\rho_b m) + \gamma$.

This result [Eq. (9)] suggests a richer dynamics: There is a competition between two small parameters δ and ε^2. When $1 \gg \varepsilon^2 \gg \delta$ $T_{mm} = |t_{mm}|^2 \approx |p|^2\delta^2(m\pi\varepsilon)^{-4}$. This is a small quantity but not necessarily smaller than $\approx \varepsilon^4$ [Eq. (5)] or $\approx \delta$ [Eq. (7)] When $\delta/\varepsilon^4 \ll 1$, most of the particles are scattered to other modes with the transmission amplitude $T_{mk} = |t_{mk}|^2 \approx (k/m)^2 \delta(\pi\sqrt{m^2-k^2})^{-1}$.

On the other hand, when $\varepsilon^2 \ll \delta \ll 1$ the transmission is close to one: $t_{mm} \approx 1 - i(m\pi\varepsilon)^2/(p\delta)$. Thus, for $\delta/\varepsilon^2 \gg 1$ the transmission is very close to $T=1$, while for $\delta/\varepsilon^2 \ll 1$, $T = T_{11} \approx |p|^2\delta^2(\pi\varepsilon)^{-4}$ is a very small quantity.

The sensitivity of the transmission [Eq. (9)] on the parameter ε suggests the possibility to detect strong resonances in an orifice with numerous defects. Resonances are very common when more than a single defect are present. In particular, when we consider two defects, the spatial distance between them is usually related to some resonance wavelengths. However, when more than one dimension is concerned, these resonances are usually quite weak (in the sense that the transmission change at the resonance is not very drastic). That is because most of the energy is usually transferred to other modes, which are present in systems that have more dimensions than one. Moreover, even when only the first mode is dominant (e.g., when low energy is concerned) the influence of the defect is usually minuscule, and can be neglected.

Taking account of the previous calculations, we find that we can overcome these difficulties when considering energies, which are very close to π^2 (in the normalized units). In this case we have only to consider the first mode, but still the defects have a strong scattering effect.

Let us consider the following system: In a thin orifice we scatter a wave with a close to threshold energy (i.e., $E \approx \pi^2$) over two impurities (defects) placed a distance L apart (see Fig. 1). In this case the scattered wave has the form

$$\psi = \psi_{\text{inc}} + \sum_j \psi_j \int d\mathbf{r}' D_j(\mathbf{r}' - \mathbf{r}_j) G(\mathbf{r}', \mathbf{r}). \tag{10}$$

The $\psi_{\text{inc}} = \sin(\pi y) e^{i\sqrt{E-\pi^2}x}$ is the incoming wave, $\psi_j(j=1,2)$ are constant, $D_j(j=1,2)$ are the defects potentials, and the integrals are taken over the whole 2D volume. The solutions to the constants ψ_j comes directly from:

$$\boldsymbol{\psi} = A^{-1}\boldsymbol{\psi}_{\text{inc}}, \tag{11}$$

where $\psi_{1,2}$ and $\psi_{\text{inc}}(\mathbf{r}_{1,2})$ are the elements of $\boldsymbol{\psi}$ and $\boldsymbol{\psi}_{\text{inc}}$, respectively, and the elements of the 2×2 matrix A are $A_{jj} = 1 - \int d\mathbf{r}' D_j(\mathbf{r}') G(\mathbf{r}')$ and $A_{ij} = -G(\mathbf{r}_i, \mathbf{r}_j) \int d\mathbf{r}' D_i(\mathbf{r}')$ for $i \neq j$.

We take the approximation $G(\mathbf{r}_1, \mathbf{r}_2) \cong -(i/2)\sin(\pi\varepsilon_1)\sin(\pi\varepsilon_2) e^{i\sqrt{E-\pi^2}L}(E-\pi^2)^{-1/2}$ (we chose $\mathbf{r}_1 = \hat{y}\varepsilon_1$ and $\mathbf{r}_2 = \hat{y}\varepsilon_2 + \hat{x}L$ for the defects locations). This is a very good approximation, because in the case under consideration, $L \approx (E-\pi^2)^{-1/2}$ (since we are interested in the resonance) and since $E\to\pi^2$, the next mode has an exponentially small contribution: $\exp(i\sqrt{E-4\pi^2}L)\approx\exp(-\sqrt{3\pi^2/(E-\pi^2)})$. After some tedious but straightforward algebra, we finally get for the scattered wave ($x>L$): $\psi=t\cdot\sin(\pi y)e^{i\delta x}$ when

$$t=[1+(c_1+c_2)+c_1c_2(1-e^{2i\delta L})]^{-1} \tag{12}$$

(compare it with Ref. 10) where $c_j\equiv\sin^2(\pi\varepsilon_j)/(i\delta d_j)$ (for $j=1,2$), $d_j\equiv(4\pi)^{-1}\ln(-\pi^2/E_j)$ and finally $E_j\equiv4e^{-\gamma}(\rho_b^j)^{-2}$ is the resonance energy of a similar defect in a free 2D space.

From Eq. (12) we learn the following: The resonance energies are the ones for which $\delta L=m\pi$ (for an integer number m). This is not a surprise, it could have been anticipated. Moreover, we could have also predict the value of the ''out-of-resonance'' (OR) transmission:

$$|t_{\rm OR}|^2\approx\frac{1}{|c_1c_2|^2}\sim\frac{\delta^4}{\sin^4(\pi\varepsilon_1)\sin^4(\pi\varepsilon_2)}. \tag{13}$$

This is merely the product of the probabilities to pass the two defects. However, the nature of the resonance (R) value is quite subtle. In an ordinary case

$$|t_R|^2\approx|c_1+c_2|^{-2}\approx\min_j\delta^2\sin^{-4}(\pi\varepsilon_j). \tag{14}$$

The ''$\min_j$'' refers to the one with the minimal value (see Ref. 10).

The magnitude of Eq. (14) is much larger than Eq. (13), but in the limit $\delta\to0$ it is still a tiny quantity.

There is, however, a case where the resonance is much larger. Consider the case where $c_1\cong-c_2$. That is, according to the definition of c_j,

$$\varepsilon_1=\varepsilon_2 \quad\text{or}\quad \varepsilon_1=1-\varepsilon_2 \tag{15a}$$

and, by the definition of d_j,

$$E_1E_2=\pi^4. \tag{15b}$$

In this special case

$$t=\frac{1}{1-c^2(1-e^{2i\delta L})} \tag{16a}$$

($c=c_1=c_2$), which implies $|t|^2\cong[1+2(2\delta L-m\pi)\eta]^{-1}$ where

$$\eta\equiv16\pi^2\frac{\sin^4\pi\varepsilon_j}{\delta^2}\,\frac{\pi^2-\ln^2(\pi^2/E_j)}{\pi^2+\ln^2(\pi^2/E_j)}. \tag{16b}$$

In that case, the resonances, which take place at $\delta L=m\pi$, correspond to an almost perfect transmission ($|t|^2\cong1$) with a very thin width (since c is very large). The resonances emphasize that even the tiniest (and the weakest) defects can lead to enormously strong resonances.

Another peculiar behavior is that in order to achieve strong resonances, the defects do not have to be identical. In an ordinary resonant tunneling system the two barriers should be the same in order to get perfect transmission. But we do not find it here, rather the contrary: first, they do not have to be at the same place [Eq. (15a)], but more important, there is no need for them to have the same characteristic energy. Instead, they should maintain [Eq. (15b)], which indicates that strong resonances and identical defects coincide only when $E_1=E_2=\pi^2$. From Eq. (16b) we also see, that this is the case where the resonance width is the narrowest.

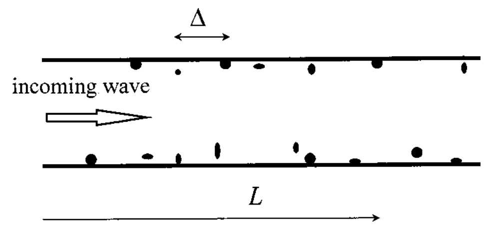

FIG. 2. Orifice with rough boundaries. Within the near-to-threshold regime, the transmission is dominated by the boundaries defects. Δ is the mean distance between defects.

Next, we consider the transmission through a rough surfaces wire (see Fig. 2) within the low-energy regime ($\omega\to\pi^2$, $\delta\to0$), i.e., the incoming energy is close to the threshold one. Let us, for example, assume that the transversal coordinates of the surface defects have the following distribution: $P(\varepsilon=\varepsilon_1)=\varepsilon_0^{-1}\exp(-\varepsilon_1/\varepsilon_0)$, where P stands for the probability and ε_0 is the characteristic distance between the defects and the boundary.

In the general case, this problem is very complicated and demands multiple scattering treatment. However, we can learn from the previous section that the $\omega\to\pi^2$ case ($\delta\to0$) is of particular simplicity. In this case the incoming wavelength is much larger than the interdefects distances. Therefore, none of the system resonances is dominant in the scattering process. Moreover, since when $\delta\to0$ the resonances are very narrow and sharp [see Eqs. (16a) and (16b)], the scattering process is insensitive to them. Actually, this is a totally out of resonance process, and hence all of the multiple interference effects can be ignored.

Therefore, we can adopt Eq. (9) to calculate the transmission through an orifice with N successive surface defects:

$$T=\prod_i|t_i|^2\cong\frac{(|p|\delta/\pi^2)^{2N}}{(\varepsilon_1\varepsilon_2\cdots\varepsilon_N)^4} \tag{17}$$

[we have conjectured here that the impurities are identical, i.e., $p\equiv\ln(-2\pi\rho_b)+\gamma$ for all of them. However, this is not a restrictive conjecture].

If we further assume that the mean distance between successive defects is a certain Δ, Eq. (17) can be approximated to

$$T\cong\exp(-L/\xi), \tag{18}$$

where L is the distance and ξ is the localization length (Fig. 2):

$$\xi\equiv-\Delta/\ln(\delta\omega_0),\quad \omega_0\equiv|p|e^{2\gamma}/\varepsilon_0^2, \tag{19}$$

and γ is the Euler constant.

Equation (18) suggests a strong localization process due to the one-dimensional characteristic behavior of the system (in the case $\omega\to\pi^2$ the process is essentially of a one-dimensional nature since the width of the wire is much smaller than the wavelength in the x direction). By virtue of Eq. (19) the localization length diverges logarithmically when approaching the threshold energy $\omega\to\pi^2(\delta\to0)$.

When the wire is empty of impurities a wave with energy lower than $\omega_{\rm th}$ cannot propagate through the wire. In the case of a single defect [Eq. (9)] we have seen a new threshold energy (will be denoted by $\omega^{i}_{\rm TH}$): when $\omega > \omega^{i}_{\rm TH} \equiv \omega_{\rm th} + \delta^{i}_{t}[\delta^{i}_{t} \cong (\pi\varepsilon)^2/|p|]$ the transmission is almost unity, but when $\omega < \omega_{\rm th} + \delta_t$ the transmission falls abruptly to a miniscule quantity [Eq. (9)]. Thus, when the wire is full of impurities, each one of them has a corresponding energy above which it is almost transparent. Therefore, the impurity with the largest distance from the boundaries (maximal ε_i) will be the one to determine the threshold of the whole wire ($\omega_{\rm TH}$).

Where there are N impurities, the probability distribution of the maximal parameter ε_i is of course[11] $P(\max_i \varepsilon_i = \varepsilon) = (N/\varepsilon_0)(1 - e^{-\varepsilon/\varepsilon_0})^{N-1} e^{-\varepsilon/\varepsilon_0}$, which leads to a threshold ($\omega_{\rm TH}$) value for the entire wire (for $L \to \infty$)

$$\omega_{\rm TH} = \int d\varepsilon P(\varepsilon)\omega^{i}_{\rm th}(\varepsilon) = \omega_{\rm th} + \delta_t ,$$

$$\text{where} \quad \delta_t \cong [(\pi\varepsilon_0)^2/|p|]\ln^2(2L/\Delta).$$

Thus, the difference between the energy threshold of the dirty wire (with many defects, i.e., $\omega_{\rm TH}$) and the clean one (without defects, i.e., $\omega_{\rm th}$) increases logarithmically with the wire length. That is, $\omega_{\rm TH(exponential)} - \pi^2 \sim \ln^2(L/\Delta)$.

In a similar way, it is straightforward to show that a Gaussian defects distribution, i.e., $P(\varepsilon = \varepsilon_1) = (2/\sqrt{\pi}\varepsilon_0)\exp[-(\varepsilon_1/\varepsilon_0)^2]$, which is much more realistic (it mimics the way corrosion penetrates the wire in a diffusion process), leads to a milder dependence on the wire length (but still logarithmic) $\omega_{\rm TH(Gaussian)} - \pi^2 \sim \ln(L/\Delta)$.

To summarize, in this work we have studied the quantum transmission through a thin wire in the low-energy regime.

(1) We showed that a single impurity (or a surface defect) can decrease the wire transmission dramatically when the particles energy is close to the threshold one. When $|p|\delta(\pi\varepsilon)^{-4} \gg 1$ (where $\delta \equiv \omega - \pi^2$ is the deviation from the threshold energy, and ε is the impurity distance from the boundary) the wire transmission is almost perfect $T = 1$, but for $|p|\delta(\pi\varepsilon)^{-4} \ll 1$ the transmission drops to $T \approx |p|^2\delta^2(\pi\varepsilon)^{-4}$.

(2) When two impurities are present we demonstrate very strong resonances. Especially in the case $E_1E_2 = \pi^4$ (the E's are the resonance energies of the corresponding impurities) the transmission $T \cong [1 + 2(2\delta L - m\pi){\rm Re}(c^2)]^{-1}$ exhibits strong resonance behavior for $\delta L = m\pi$.

(3) We calculate the transmission through a rough-boundaries wire. The transmission then looks like $T \cong \exp(-L/\xi)$ where $\xi = -\Delta/\ln(\delta\omega_0)$ (Δ and ω_0 characterize the impurities and L is the wire length), i.e., decays exponentially with the wire length. We also show, that the threshold energy for transmission increases logarithmically with the wire length $\omega_{\rm TH} - \pi^2 \sim \ln(L/\Delta)$.

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