Universal conductance reduction in a quantum wire

Er’el Granot *

Department of Electrical Engineering, College of Judea and Samaria, Ariel 44837, Israel

(March 22, 2022)

Even a single point defect in a quantum wire causes a conductance reduction. In this paper we prove (without any approximations) that for any point impurity this conductance reduction in all the sub-bands is exactly \(2e^2/h\). Moreover, it is shown that in the case of a surface defect, not only is the conductance minimum independent of the defect characteristics, but the transmission matrix also converges to universal (defect-independent) values. We also discuss particle confinement between two arbitrarily weak point defects.

PACS: 73.40G and 73.40L

The conductance of a quantum wire is quantized. When the quantum wire is contaminated by impurities, this quantization disappears. However, at the sub-bands’ threshold energies, there is always a reminiscence of the quantization. Namely, when the Fermi level is at the band bottom (the threshold energy) of the \((m+1)\)th sub-band, the conductance is exactly \(2me^2/h\). This feature is independent of the impurities’ strength. Many works validate this finding [1–3]. Recently, however, it has been found [1–4] that below the threshold energy of the \(m\)th mode, even a single defect is responsible for an unexpectedly large reduction in conductance: the weaker the impurity, the closer the dip to the threshold energy. The proximity to the pinned (i.e., defect-independent) energy level makes this reduction quite odd. Chu and Sorbello [1] attributed this feature to multiple scattering due to the defect’s presence; however, it is shown that it is always (for any point defect) equal to exactly \(2e^2/h\) and prove that it is always (for any point defect and in all the sub-bands) equal to exactly \(2e^2/h\). This reduction is distributed unevenly among the propagating modes.

In this paper we calculate the conductance reduction exactly and prove that it is always (for any point defect and in all the sub-bands) equal to exactly \(2e^2/h\). This reduction is distributed unevenly among the propagating modes.

For such a system (a point impurity in a quasi-1D wire, see Fig.1), the 2D Schrödinger equation is

\[
\nabla^2 \psi + (\omega - V) \psi = -D (r - r_0) \psi
\]

(1)

(hereinafter we use the units \(\hbar = 2m_0 = 1\), where \(m_0\) is the electron’s mass). \(V\) is the potential of the wire walls (\(V = 0\) inside the wire and \(V = \infty\) outside it), \(D\) is the defect potential and \(r_0 = \xi \hat{y}\) is the impurity location. Since the defect has the properties of a point-like impurity, the right-hand term of the Schrödinger equation can be written \(D (r - r_0) \psi (r_0)\) [6], which allows for an exact scattering solution.

Let us denote the incident wave by \(\psi_{inc}\). Then, taking advantage of the point-like nature of the impurity, the scattered wave function due to the defect’s presence can be written [7]

\[
\psi_{sc} = \psi_{inc} - \frac{\psi_{inc} (r_0) \int dr' D (r' - r_0)}{1 + \int dr' G^+ (r', r_0) D (r' - r_0) G^+ (r, r_0)} G^+ (r, r_0)
\]

(2)

where \(G^+ (r_1, r_2)\) is the ”outgoing” 2D Green function of the geometry (the wire) and \(\psi_{inc}\) is the incident wave (a homogeneous solution). It should be noted that eq. 2 is an exact solution. However, if the impurity were not an ideal point impurity, this equation would be a first-order approximation in the asymptotic solution \(|r| \to \infty\.

The Green function for the given wire geometry takes the form:

\[
G (r, r') = i \sum_{n=1}^{\infty} \frac{\sin(n\pi y) \sin(n\pi y')}{k_n} \e^{i k_n |x - x'|}
\]

(3)

where \(r = x \hat{x} + y \hat{y}\), \(r' = x' \hat{x} + y' \hat{y}\) and \(k_n = \sqrt{\omega - (n\pi)^2}\) is the effective wavenumber. Hereinafter, the length parameters are normalized to the wire’s width.

FIG. 1. A 2D wire with a single point defect (the black dot)

Choosing the right potential for the impurity is a very tricky business as can be understood from the literature

ere@yosh.ac.il
[1,3,4,6,8,9] (see also ref.17 of [8]). A simple 2D delta function (2DDF), which is a natural candidate to represent a point impurity (like in 1D), i.e., \(\delta(x)\delta(y)\), does not scatter (its cross section is zero), and therefore cannot be used.

Throughout this article we use the Impurity D Function (IDF) that was first presented by Azbel [6]. However, since in our wire’s geometry the problem’s symmetry is Cartesian rather than radial, we choose the following IDF:

\[
D(r) = \lim_{\rho \to 0} \frac{2\sqrt{\rho} \delta(x)}{\rho \ln(\rho)} \exp\left(-\frac{y^2}{\rho^2}\right),
\]

Unlike the 2DDF, this potential, which is infinitely shallower, does scatter [6]. The de Broglie wavelength of the impurity’s bound state is \(\lambda_B = \pi \rho_0 \exp(\gamma/2)/2\). This is the only parameter that characterizes the impurity, and therefore eq. 4 can be used to mimic any impurity with the same de Broglie wavelength, the width of which is much smaller than \(\lambda_B\) (i.e., a point defect).

On the face of it, the solution is straightforward: all that is needed is to substitute eqs. 4 and 3 into eq. 2. However, the Green function has a logarithmic singularity at \(|r-r'| \to 0\). Here is where the impurity’s width \(\rho\) plays a major part, and the limit \(\rho \to 0\) should be approached with great caution. Therefore, we first solve the integral for a finite \(\rho\) and only then evaluate the limit.

We assume that the incident wave is the \(n\)th mode, and that the incident energy is close to the \(n\)th threshold energy (i.e., \(\omega \simeq (m\pi)^2\)), giving

\[
\psi_{inc}(r) = \sin(n\pi y) \exp(ik_n x).
\]

By using the following relation

\[
\int dy \sin(n\pi y) \exp\left[-(y-\varepsilon)^2/\rho^2\right] = \rho \sqrt{\pi} \sin(n\pi \varepsilon) \exp\left[-(n\pi\rho/2)^2\right]
\]

we find the solution \((x > 0)\)

\[
\psi_{sc}(r) = \sum_{l=1}^{\infty} (\delta_{nl} - A_{nl}) \sin(l\pi y) \exp(ik_l x)
\]

where \(\delta_{nl}\) is the Kronecker delta,

\[
A_{nl} \equiv \frac{\sin(n\pi \varepsilon) \sin(l\pi \varepsilon)}{ik_l} \left[\ln(\rho_0/\bar{\rho}) + \sum_{n'=m}^{\infty} \frac{\sin^2(n'\pi \varepsilon)}{k_{n'}^2}\right]
\]

and \(\bar{\rho}\) is some length scale which depends on the impurity’s location \(\varepsilon\), the incident energy \(\omega\) and \(m\):

\[
\ln(\bar{\rho}) \equiv \lim_{\rho \to 0} \left\{ \ln \rho + 2\pi \sum_{n'=m+1}^{\infty} \frac{\sin^2(n'\pi \varepsilon)}{qa'_{n'}} e^{-(n'\pi \rho/2)^2} \right\}
\]

where \(q_n \equiv \sqrt{(n\pi)^2 - \omega}\).

The conductance can be evaluated by the Landauer equation [10]

\[
G = \frac{1}{\pi} \sum_{n,l} T_{nl}
\]

where

\[
T_{nl} = \begin{cases} |1 - A_{nn}|^2 & n = l \\ |A_{nl}|^2 & n \neq l \end{cases}
\]

are the transmission coefficients. Clearly, at the threshold energies where \(\omega = (m\pi)^2\), the coefficients vanish, \(A_{nl} = 0\) for any \(n,l < m\), and therefore

\[
G = \frac{1}{\pi}(m-1)
\]

independent of the impurity, as has been shown in previous works [1–3].

However, eq. 8 allows us to calculate the minima of the conductance as well. The minima are obtained when the imaginary part of eq. 8 vanishes, i.e., when

\[
\frac{\ln(\rho_0/\bar{\rho})}{2\pi} = \frac{\sin^2(n\pi \varepsilon)}{q_m},
\]

and thus

\[
A_{nl}^{min} = \left[\sum_{j=m}^{\infty} \frac{\sin^2(j\pi \varepsilon)}{\sin(n\pi \varepsilon) \sin(l\pi \varepsilon)} k_j\right]^{-1}.
\]

Using eqs. 10, 11 and 14, at the minimum points \((G = G_m)\)

\[
G_m = \frac{1}{\pi} \sum_{n,l<m} \left\{ \delta_{nl} - \left[\sum_{j<m} \frac{\sin^2(j\pi \varepsilon)}{\sin(n\pi \varepsilon) \sin(l\pi \varepsilon) k_j}\right]\right\}^2
\]

This complicated expression can be considerably simplified: with the following definition

\[
\sigma \equiv \sum_{j<m} \frac{\sin^2(j\pi \varepsilon)}{k_j}
\]

eq 15 can be rewritten

\[
\pi G_m = \sum_{n<m} \frac{1 - 2 \sigma}{\sigma^2} \sum_{n=1}^m \frac{\sin^2(n\pi \varepsilon)}{k_{n} k_{n'}}
\]

The first term of eq. 17 is equal to \(m-1\), the second and third terms are, by definition, equal to 2 and 1, respectively, and therefore the minimum conductance near the \(m\)th threshold energy is simply

\[
G_m = \frac{1}{\pi}(m-2)
\]
which, again, is independent of the defect’s properties (location and strength). Any point defect will exhibit the same conduction transition, from the minima (eq. 18) to the maxima (eq. 12). Hence, the defect reduced the conductance by exactly $\Delta G \equiv G_{\text{max}} - G_{\text{min}} = \pi^{-1} (= 2\varepsilon^2/h)$ in every band (see Fig. 2).

In general, eq. 8 is considerably simplified when the defect is close to the boundary, i.e., $\varepsilon \ll 1$. In that case (near the $m$th band)

$$A_m \simeq \left[ \sum_{j < m} \frac{j^2}{nl} \sqrt{\frac{m^2 - j^2}{m^2 - j^2}} + i\pi \frac{\sqrt{m^2 - j^2}}{nl} \left( \Delta^{-1} - \frac{m^2}{q_m} \right) \right]^{-1}$$

and

$$\Delta \equiv 2\pi \frac{(\pi \varepsilon)^2}{ln(\rho_0/\varepsilon C)}$$

where $C \equiv 4 \exp[\gamma/2 + Ci(\pi)] \simeq 5$ is a numerical constant ($\gamma$ is the Euler constant and $Ci$ is the cosine integral).

Hence, the reduction takes place at the following energies

$$\omega_m^* \simeq (m\pi)^2 - m^4 \Delta^2$$

These energies depend on the defect’s characteristics (via $\Delta$) but the *amount of the reduction* does not.

In the limit $\varepsilon \to 0$, i.e., when the defect is a surface defect, another universality appears: not only is the conductance independent of the defect characteristics but the transmission matrix is also defect-independent. At the minima, the transmission coefficients converge to the limits

$$\lim_{\varepsilon \to 0} T_{l\neq m} = \left| 1 - \left[ \sum_{j < m} \frac{j^2}{n^2} \sqrt{\frac{m^2 - n^2}{m^2 - j^2}} \right]^{-1} \right|^2$$

which are merely pure numbers, in which no reminiscence of the defect’s characteristics is left out.

The fact that the reduction in conductance is independent of the band number is not trivial since this reduction is distributed *unevenly* among all the propagating modes. Therefore, the first reduction, just below the $m = 2$ sub-band is a special case. At this energy the conductance is reduced to zero, and is a consequence of a single mode (the first one), which is totally reflected. This is the only point at which a propagating mode is totally reflected by a single point defect (note that unlike ref. [11], we obtained this result without any approximations). This unique energetic place can be used to create a bound state in the continuum, simply by binding it between two totally reflecting defects. At this energy Kim and Satanin [9] also found a bound state in the continuum, but for the problematic 2DDF model. The presence of an additional defect can create zero transmission regions at higher energies, and therefore with more defects it becomes possible to bind particles at higher sub-bands. In the following we will evaluate the minimum distance between two defects, which allows for such binding.

FIG. 3. The probability density of the bound state

By adding another defect, the Schrödinger equation will look like

$$\nabla^2 \psi + (\omega - V) \psi = -D (r - r_1) \psi - D (r - r_1 - L\hat{x}) \psi.$$ (24)

It is then clear that if the defects are located at the same distance from the boundary and the distance between them, $L$, is extremely large ($L \gg 1$ so the inter-scattering can be ignored) and maintains $L = \frac{n\pi}{\sqrt{\omega^2 - \pi^2}} \simeq \frac{n}{\sqrt{\pi}}$ (where $n$ is an integer, and $\omega^2_*$ can be evaluated from eq. 21 for $m = 2$ when the defects are very far apart $n \to \infty$), the system will hold a bound eigen state with the eigen energy that corresponds to $\omega^2_*$ (when the distance between them is finite, the binding energy increases). In Fig. 3, the probability density of such a bound eigenstate (for $\varepsilon = 10^{-3}$) is shown.
It is well known that in wave dynamics only an infinite barrier (either high or long) can totally reflect the incident wave. Therefore, in principle, only infinite barriers can confine a quantum state. So how is it possible for only two point scatterers, which can be arbitrarily weak, to confine an energetically bound state in the continuum? The answer is that what really confines the quantum particle is the infinite wire’s boundaries rather than the point scatterers. All the scatterers need to do is to deviate the particle’s trajectory a little.

A classical analogy to such a confinement is shown in Fig. 4. Two opposite planes, which have an arbitrary small slope, can confine an energetic classical particle like these slopes.

One should therefore expect that the strength of the defect will determine a minimum distance within which it is possible to confine a particle.

After some tedious, albeit straightforward calculations, it can be shown that a bound state in the $M$th propagating sub-band (i.e., $\{M+1\}^2 > \omega > (M\pi)^2$) should satisfy the following coupled equations (the second equation holds only in the limit $\rho \to 0$):

$$\sum_{n=1}^{M} \frac{\sin^2(n\pi\varepsilon)}{k_n} \sin^2(k_n L/2) = 0 \quad (25)$$

$$\ln(\rho_0/\rho) = \sum_{n=M+1}^{\infty} \frac{\sin^2(n\pi\varepsilon)}{q_n} \left[ e^{-(n\pi\rho/2)^2} - e^{-q_n L} \right]. \quad (26)$$

Since all the terms in eq. 25 are non-negative, a solution is possible only when all the terms vanish. For an arbitrary $\varepsilon$ (non-rational) we should demand

$$\sqrt{\omega - n_1^2} L = 2n_1 \pi,$$

$$\sqrt{\omega - (2\pi)^2} L = 2n_2 \pi,$$

$$\vdots$$

$$\sqrt{\omega - (M\pi)^2} L = 2n_M \pi,$$

where $n_1, n_2, \ldots, n_M$ are integers. Eq. 26 is reduced, in the limit of a surface defect $\varepsilon \to 0$, to a simple expression

$$L = -\frac{\ln\{1 - q_{M+1}/(M + 1)^2\Delta\}}{q_{M+1}}. \quad (28)$$

Hence, the minimum distance within which it is possible to confine the bound state is inversely proportional to $\Delta$:

$$L_{\text{min}} = 1/(M + 1)^2 \Delta. \quad (29)$$

To summarize, we calculated the transmission and conductance of a quantum wire which was contaminated by a single defect. We showed that the reduction in the conductance in all the sub-bands is *totally universal* (independent of the defect’s characteristics), and is always equal to $2e^2/h$. Moreover, we showed that when the point defect is a surface impurity, the transmission coefficients at the minima converge to *universal numbers* (and again, are independent of the defect). We used this result to show that it is possible to confine an eigenstate in the *continuum* of the quantum wire between two totally reflecting defects, and to show the limitations enforced upon it.

It should be stressed that while the discussion was focused on quantum wires, this effect can occur in any waveguide with a single point scatterer: acoustical waveguide, electromagnetic waveguide, optical waveguide, etc.

[1] C.S. Chu and R.S. Sorbello, Phys. Rev. B 40 5941 (1989)
[2] P.F. Bagwell, Phys. Rev. B 41 10354 (1990)
[3] Y.B. Levinson, M.I. Lubin, and E.V. Sukhorukov, Phys. Rev. B 45, 11936 (1992).
[4] E. Tekman and S. Ciraci, Phys. Rev. B 42, 9098 (1990)
[5] J.U. Nöckel and A.D. Stone, Phys. Rev. B 50, 17415 (1994)
[6] M. Ya. Azbel, Phys. Rev. B 43 2435 (1991); Phys. Rev. B 43 6717 (1991); Phys. Rev. Lett. 67, 1787 (1991).
[7] E. Granot and M.Ya. Azbel, Phys. Rev. B 50, 8868 (1994); J. Phys. Condens. Matter 11, 4031 (1999).
[8] P.F.Bagwell, and R. Lake, Phys. Rev. B 46, 15329 (1992)
[9] C.S. Kim and A.M. Satanin, Physica E 4, 211 (1999).
[10] R. Landauer, IBM J. Res. Dev. 1, 223 (1957); 32, 306 (1988).
[11] S.A. Gurvitz and Y.B. Levinson, Phys. Rev. B 47, 10578 (1993)