Transmission coefficient for a point scatterer at specific energies is affected by the presence of the scatterer but independent of the scatterer's characteristics

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We calculate the exact transmission coefficients of a quantum wire in the presence of a single point defect at the wire's cutoff frequencies. We show that at these frequencies while the conductance pattern (i.e., the scattering) is strongly affected by the presence of the defect, the pattern is totally *independent* of the defect's characteristics (i.e., the defect that caused the scattering cannot be identified from that pattern). The change in the conduction pattern can cause universal attraction and/or repulsion forces between two parallel conducting wires.

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One of the most common ways to investigate the inner structure of a system is to perform scattering studies. That is, by looking at the scattering *pattern* (the way waves are distributed in space) one can cull some notion about the scatterer that was the cause of the specific scattering pattern. Our experience shows that every scatterer has a different scattering pattern. That explains the ubiquity of scattering techniques in the diagnostic world: for crystallographic studies, x rays are used; visible light is usually used to detect molecule energy levels; ultrasound waves are commonly used for embryo imaging, etc.

In this paper, we discuss a case of a narrow wire at specific energies in which our experience (that every scatterer has a different scattering pattern) fails. In this case, the scatterer has a strong influence on the dynamics of the system, both in terms of conductance (either high or low) and on the conduction pattern. However, the conductance and the scattering pattern are *totally independent* of the scatterer. The scatterer's elusive conduct can be phrased: *One can see the scatterer's "footprints" (its strong influence), but cannot see its "fingerprints" (anything that may assist to characterize it)*.

When we think of a small and weak scatterer, the thing we usually have in mind is a scatterer whose influence on scattering is negligible. One of the reasons for this is that we are accustomed to a 3D world. In this case, the cross section is $\sigma \sim V^2$ (see Ref. 1), where V is the scatterer strength (potential), i.e., it vanishes with scatterer potential. In 1D, however, this is definitely not the case. It is well known that when the incident particles' energy is considerably lower (see below) than the scatterer's strength (i.e., the scatterer's potential), most of the incident particles are reflected from the scatterer, i.e., the scattering coefficient is large regardless of scatterer's weak potential (so long, of course, as the particles' energy is lower than the scatterer's potential). This behavior can be presented easily in the case of a weak scatterer, in which the reflection coefficient is related to the 1D scattering cross section. By using the term "weak scatterer" (or "shallow scatterer") we refer to the case in which its strength (its weak potential ΔV) and its width (L) satisfy $\sqrt{\Delta V}L \ll 1$ (with the units $\hbar = 2m = 1$). In this case, the reflection coefficient maintains

$$R \simeq \frac{1}{1 + 4\omega/(\Delta V L)^2}, \tag{1}$$

where ω is the energy of the incident particles. One can easily be convinced, though quite surprisingly, that the extreme case of the *infinitely shallow* potential barrier is actually the 1D delta function. That is, for the potential barrier $\alpha\delta(x)$ (or the limit of $\Delta V = \alpha/L$ for $L \to 0$), the reflection coefficient reads

$$R = \frac{1}{1 + 4\omega/\alpha^2} \tag{2}$$

(notice that now this is an equation and not merely an approximation). Equations (1) and (2), despite their simplicity, hold some behaviors, which cannot be found in 3D scattering. These behaviors can be summarized in three points:

(1) The reflection coefficient *increases* when the energy decreases.

(2) The scattering is strong (high scattering coefficient) despite the scatterer's "weakness" (weak potential).

(3) The scattering for $\omega \to 0$ is *independent* of the scatterer (it does not depend on α).

The third point is probably the most peculiar, since it contradicts our statement that each scatterer has a distinct scattered wave function. However, in 1D this feature is hardly interesting since it is valid only for zero incident particle energy ($\omega = 0$). A particle with zero energy has little chance of even reaching the scatterer. In quasi-1D systems, the situation can be quite different.

In the case of the thin wire, for example, there are an infinite number of threshold (cutoff) energies. When the incident particles have exactly the cutoff energy of the mth mode, no energy is transferred to it (to the mth mode), since the momentum (or the k vector) of this mode in the propagation direction is zero. Therefore, it makes sense to expect to find all the peculiarities of the 1D case, even in a 2D wire, near the threshold energies.

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

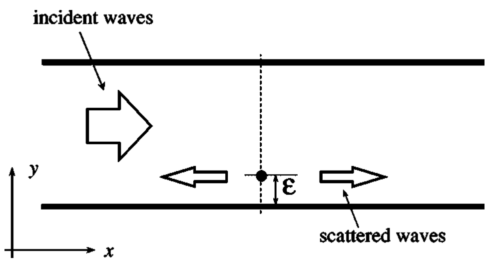

FIG. 1. A 2D wire with a single point defect (black dot).

$$\nabla^2\psi + (\omega - V)\psi = -D(\mathbf{r}-\mathbf{r}_0)\psi \tag{3}$$

(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 $\mathbf{r}_0=\varepsilon\hat{\mathbf{y}}$ is the impurity location (see Fig. 1). Since the defect has the properties of a pointlike impurity, the right-hand term of the Schrödinger equation can be written $D(\mathbf{r}-\mathbf{r}_0)\psi(\mathbf{r}_0)^2$, which allows for an exact scattering solution.

Let us assume that we hit the impurity with the incident wave $\psi_{\rm inc}$. Taking advantage of the pointlike nature of the impurity, the scattered wave function due to the defect is[3–5]

$$\psi_{\rm sc} = \psi_{\rm inc} - \frac{\psi_{\rm inc}(\mathbf{r}_0)\int d\mathbf{r}' D(\mathbf{r}'-\mathbf{r}_0)}{1+\int d\mathbf{r}' G^+(\mathbf{r}',\mathbf{r}_0)D(\mathbf{r}'-\mathbf{r}_0)} G^+(\mathbf{r},\mathbf{r}_0), \tag{4}$$

where $G^+(\mathbf{r}',\mathbf{r}'')$ is the "outgoing" 2D-Green function of the geometry (the wire). It should be noted that Eq. (4) 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 $|\mathbf{r}\to\infty|$. The Green function for the given wire geometry takes the form

$$G(\mathbf{r},\mathbf{r}') = i\sum_{n=1}^{\infty}\frac{\sin(n\pi y)\sin(n\pi y')}{\sqrt{\omega-(n\pi)^2}}\exp[i\sqrt{\omega-(n\pi)^2}|x-x'|] \tag{5}$$

where $\mathbf{r}\equiv x\hat{x}+y\hat{y}$ and $\mathbf{r}'\equiv x'\hat{x}+y'\hat{y}$. Hereinafter, the length parameters are normalized to the wire's width.

Choosing the right potential for the impurity is a very tricky business as can be understood from the literature.[6–12] A simple 2D delta function (2DDF), which is a natural candidate to represent a point impurity (such as in 1D), i.e., $\delta(x)\delta(y)$, does not scatter (its cross section is zero, see the discussion in Ref. 17 of Ref. 13). Throughout this paper we use the impurity D function (IDF) that was first presented by Azbel.[2] However, since in our wire's geometry the problem's symmetry is Cartesian rather than radial, we choose the following IDF (it should be stressed, however, that a qualitatively similar effect will appear even for a finite-size, but small, scatterer):

$$D(\mathbf{r}) \equiv \lim_{\rho\to 0}\frac{2\sqrt{\pi}\delta(x)}{\rho\ln(\rho/\rho_0)}\exp(-y^2/\rho^2). \tag{6}$$

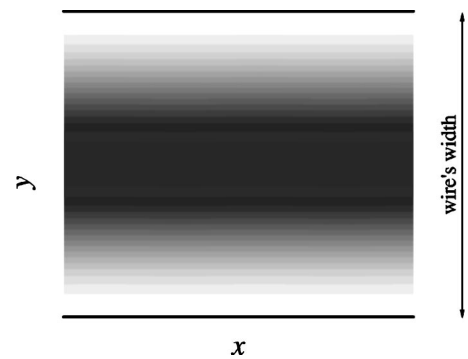

FIG. 2. The probability density distribution in the wire for $n=1$ and $\omega=(2\pi)^2$ in the absence of the point defect.

Unlike the 2DDF, this potential, which is infinitely shallower than the 2DDF, does scatter.[2] The de Broglie wavelength of the impurity's bound state is $\lambda_B=\pi\rho_0\exp(\gamma/2)/2$ (where $\gamma\simeq 0.577$ is the Euler constant). This is the only parameter that characterizes the impurity, and therefore Eq. (6) can be used to mimic any impurity with the same de Broglie wavelength, where its width is much smaller than λ_B.

On the face of it, the solution is straightforward: simply to substitute Eqs. (6) and (5) into Eq. (4). The problem is that the Green function has a logarithmic singularity at $|\mathbf{r}-\mathbf{r}'|\to 0$. Here is where the impurity's width ρ plays a major part, and the limit $\rho\to 0$ should be taken with great caution. Therefore, we first solve the integral for a finite ρ and only then evaluate the limit.

Let us assume that the incident wave is the nth mode, and that the incident energy is close to the mth threshold energy [i.e., $\omega\simeq(m\pi)^2$]. Therefore,

$$\psi_{\rm inc}(\mathbf{r}) = \sin(n\pi y)\exp[i\sqrt{\omega-(n\pi)^2}x]. \tag{7}$$

The probability density of Eq. (7) is presented in Fig. 2 for $n=1$ and $m=2$.

By using the following relation,

$$\int_{-\infty}^{\infty} dy\,\sin(n\pi y)\exp[-(y-\varepsilon)^2/\rho^2] = \rho\sqrt{\pi}\sin(n\pi\varepsilon)\exp[-(n\pi\rho/2)^2], \tag{8}$$

we find the solution (for $x>0$)

$$\psi_{\rm sc}(\mathbf{r}) = \sum_{l=1}^{\infty}(\delta_{nl}-A_{nl})\sin(l\pi y)\exp[i\sqrt{\omega-(l\pi)^2}x] \tag{9}$$

where δ_{nl} is the Kronecker delta and

$$A_{nl} \equiv \frac{\sin(n\pi\varepsilon)\sin(l\pi\varepsilon)}{i\sqrt{\omega-(l\pi)^2}\left(\frac{\ln(\rho_0/\bar{\rho})}{2\pi}+\sum_{n'\leq m}\frac{\sin^2(n'\pi\varepsilon)}{i\sqrt{\omega-(n'\pi)^2}}\right)} \tag{10}$$

and $\bar{\rho}$ is some length scale which depends on the impurity's location (ε), the incident energy ω and m:

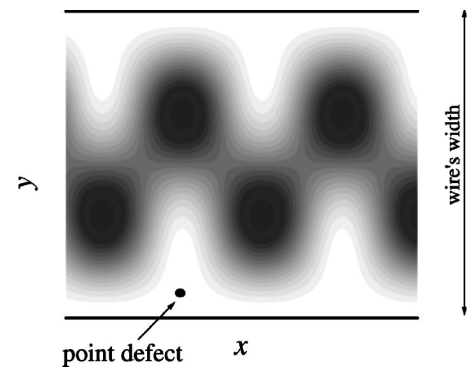

FIG. 3. The probability density distribution in the wire for $n=1$ and $\omega=(2\pi)^2$ when the point defect is present.

$$\ln(\overline{\rho}) \equiv \lim_{\rho\to 0}\left\{ \ln\rho + 2\pi \sum_{n'=m+1}^{\infty} \frac{\sin^2(n'\pi\varepsilon)}{\sqrt{(n'\pi)^2-\omega}} e^{-(n'\pi\rho/2)^2} \right\}. \tag{11}$$

In this paper we discuss the case where $\omega \simeq (m\pi)^2$ for any integer m [though the figures are focused on the case $\omega \simeq (2\pi)^2$, i.e., $m=2$]. In this particular case only the nth mode (the incident mode) and the mth one have a considerable influence on the scattering,

$$\psi_{\mathrm{sc}} \simeq \psi_{\mathrm{inc}} - \frac{\sin(n\pi\varepsilon)}{\sin(m\pi\varepsilon)} \frac{\sin(m\pi y) e^{i\sqrt{\omega-(m\pi)^2}|x|}}{1+i\sqrt{\omega-(m\pi)^2}/\Delta_m}, \tag{12}$$

where

$$\Delta_m^{-1/2} \equiv \frac{\ln(\rho_0/\overline{\rho})}{2\pi\sin^2(m\pi\varepsilon)} - i\sum_{n'<m} \frac{\sin^2(n'\pi\varepsilon)}{\sin^2(m\pi\varepsilon)} \frac{1}{\pi\sqrt{m^2-n'^2}}. \tag{13}$$

The scattered wave function, i.e., Eq. (12), depends on the scatterer's parameter (ρ_0) only via Δ_m. Therefore, when

$$[\omega-(m\pi)^2]/\Delta_m \ll 1, \tag{14}$$

one finds the following.

(1) When the energy is not close to the threshold energy, the scattering is negligible; as we get closer to the threshold energy, the scattering increases.

(2) The scattering coefficient is large (can have *any* value) regardless of the vanishing cross section of the scatterer.

(3) Near the threshold energies, the scattering is *independent* of the scatterer (it does not depend on the scatterer's parameter).

Again, the most bizarre behavior is the third one, which is manifested in the limit $\omega \to (m\pi)^2$ of Eq. (12) (see Fig. 3):

$$\psi_{\mathrm{sc}} = \psi_{\mathrm{inc}} - \frac{\sin(n\pi\varepsilon)}{\sin(m\pi\varepsilon)}\sin(m\pi y). \tag{15}$$

Equation (15), which presents the scattering of the nth mode, when its energy is equal to the threshold energy of the mth one, can be generalized for a wire with an arbitrary (but uniform) cross section,

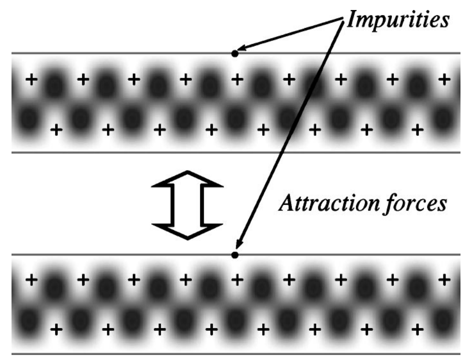

FIG. 4. The change in the scattering pattern can cause a net attraction between two conducting wires.

$$\psi_{\mathrm{sc}} = \chi_n(y) e^{i\sqrt{\omega_m-\omega_n}x} - \frac{\chi_n(\varepsilon)}{\chi_m(\varepsilon)}\chi_m(y), \tag{16}$$

where $\chi_n(y)$ is the transversal eigenstates of the wire, with the corresponding eigenenergies ω_n.

While Eq. (12) is an approximation, Eqs. (15) and (16) are totally accurate for *any point impurity*, and at any impurity's location.

In the case of a surface impurity, i.e., $\varepsilon \to 0$ (or $\varepsilon \to 1$), Eq. (12) is reduced to an even simpler expression

$$\psi_{\mathrm{sc}} \simeq \psi_{\mathrm{inc}} \mp \left(\frac{n}{m}\right) \frac{\sin(m\pi y) e^{i\sqrt{\omega-(m\pi)^2}|x|}}{1+i\sqrt{\omega-(m\pi)^2}/\Delta_m}, \tag{17}$$

where

$$\Delta_m^{-1/2} \simeq \frac{\ln(\rho_0/C\varepsilon)}{2\pi(m\pi\varepsilon)^2} \tag{18}$$

and

$$C \equiv 4\exp[\gamma/2 - \mathrm{Ci}(\pi)] \simeq 5 \tag{19}$$

is a numerical constant (Ci is the cosine integral). The upper sign (minus) in Eq. (17) stands for impurity at the lower boundary $\varepsilon \ll m^{-1}$ while the plus implies an upper boundary impurity $1-\varepsilon \ll m^{-1}$ [in this case the ε should be replaced by $1-\varepsilon$ in Eq. (18)].

Thus, at the threshold energy, i.e., $\omega=(m\pi)^2$,

$$\psi_{\mathrm{sc}} = \sin(m\pi y) e^{i\pi\sqrt{m^2-n^2}x} \mp \left(\frac{n}{m}\right)\sin(m\pi y). \tag{20}$$

That is, in the case of a *surface* impurity then close enough to the threshold energies [i.e., when Eq. (20) holds], the scattering is also independent of the impurity's *location*. Any impurity's characteristics have faded away near the threshold energies. Equation (20) does not reflect any feature of the scatterer: it depends neither on its strength nor on its location.

The most direct way to measure the effect is by an interference experiment as suggested in Ref. 4. However, in the case of a conducting wire the effect is also accompanied by electric forces. In the case presented in Fig. 4, for example, two identical conducting wires are placed one next to the other with a single impurity in both. When the incident particles' energy is exactly at the second cutoff level (i.e., $m=2$), and the incoming function is equal to Eq. (7) with $n=1$, the scattering pattern that appears reorganizes the charge distribution along the wire, causing a net attraction forces between the wires. Clearly, the attraction can easily be flipped into repulsion by simply positioning one of the impurities at the opposite side of the wire. Due to the universality, the forces will depend on the impurities' presence but not on their characteristics.

The forces between the wires decay exponentially with the distance between them, where the decay length is of the order of the wavelength. When the incident particles's energy is lower than the second threshold energy the forces will disappear.

It was shown in the literature (see, for example, Ref. 6) that at the threshold energies, the conductance is totally quantized and is independent of the point defects; however, here we show two additional results: the scattering coefficient is not a negligible quantity, it does not affect the conductance but it does distort the conduction *pattern* (i.e., it changes the scattered wave function), and, at the same time, that this severe distortion is *independent of the scatterer that caused it*.

It should be stressed that while the discussion was focused on quantum wire, this effect can occur in any waveguide with a single point scatterer: acoustical waveguide, electromagnetic waveguide, optical waveguide, etc. Moreover, although for convenience we used an IDF as the defect potential, the same analysis can easily be generalized to any chosen point scatterer.

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[1] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970).
[2] M. Ya. Azbel, Phys. Rev. B **43**, 2435 (1991); **43**, 6717 (1991); Phys. Rev. Lett. **67**, 1787 (1991).
[3] E. Granot and M. Ya. Azbel, Phys. Rev. B **50**, 8868 (1994).
[4] E. Granot, Phys. Rev. B **60**, 10 664 (1999); **61**, 11 078 (2000).
[5] P. F. Bagwell, J. Phys.: Condens. Matter **2**, 6179 (1990).
[6] C. S. Chu and R. S. Sorbello, Phys. Rev. B **40**, 5941 (1989).
[7] A. Kumar and F. Bagwell, Phys. Rev. B **43**, 9012 (1991).
[8] P. F. Bagwell, Phys. Rev. B **41**, 10 354 (1990).
[9] Y. B. Levinson, M. I. Lubin, and E. V. Sukhorukov, Phys. Rev. B **45**, 11 936 (1992).
[10] S. A. Gurvitz and Y. B. Levinson, Phys. Rev. B **47**, 10 578 (1993).
[11] E. Tekman and S. Ciraci, Phys. Rev. B **42**, 9098 (1990).
[12] C. S. Kim and A. M. Satanin, Physica E (Amsterdam) **4**, 211 (1999).
[13] P. F. Bagwell and R. K. Lake, Phys. Rev. B **46**, 15 329 (1992).