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Asymmetric features in the resistivity of clean quasi-one-dimensional systems: Fano resonances or non-Born effects?

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Complex asymmetric features in resistivity of clean quasi-one-dimensional systems (e.g., carbon nanotubes and nanoconstrictions in 2D semiconductor heterostructures) as a function of chemical potential E_F were observed experimentally [1, 2]. Usually they were attributed to Fano resonances [3], described by formula

$$\rho(E_F) \propto \frac{(E_F - E_{\text{res}} + q\Gamma/2)^2}{(E_F - E_{\text{res}})^2 + (\Gamma/2)^2}. \quad (1)$$

In this paper we show that formula (1) can not describe the entire zoo of resistivity shapes that arise already in the simple model of conducting tube of radius R with short-range impurities at low concentration n. Density of states and resistivity of a clean tube demonstrate Van Hove singularities arising at bottoms of each of one-dimensional subbands of transverse quantization. As it was shown in [4], taking scattering into account within the self-consistent Born approximation smears the singularity. Below we demonstrate that these results are inapplicable for the case of sufficiently low $n \ll n_c$ where n_c is some crossover concentration which is determined in what follows. We evaluate the resistivity of the tube in the simplest "diffusion approximation" – via the Kubo formula in Drude approximation. Dimensionless parameters $n = (2\pi R)^2 n_2$ (where n_2 is two-dimensional concentration of impurities on the surface of the tube) and λ (dimensionless scattering amplitude) are assumed to be small: $n, |\lambda| \ll 1$. Away from Van Hove singularity, the density of states ν and resistivity ρ of the tube can be trivially expressed through the density of states ν_0 and the scattering time τ_0 of electrons in the 2D metal constituting the surface of the tube:

$$\nu = \nu_0 = m^* R,\ \rho = \rho_0 = \frac{1}{e^2 \varepsilon_F \tau_0},\ \frac{1}{\tau} = \frac{1}{\tau_0} = 2n\left(\frac{\lambda}{\pi}\right)^2$$

where m^* is effective mass of an electron. When the Fermi level comes close (but not too close, see below!) to Van Hove singularity, expressions for the density of states and the scattering time change:

$$\nu(\varepsilon) = \nu_0\left(1 + \frac{\theta(\varepsilon)}{\pi\sqrt{\varepsilon}}\right), \quad \frac{1}{\tau(\varepsilon)} = \frac{1}{\tau_0}\frac{\nu(\varepsilon)}{\nu_0}. \quad (2)$$

Here dimensionless parameter $\varepsilon = 2m^* R^2 (E_F - E_N)$ is proportional to distance between Fermi level and the bottom E_N of resonant subband of transverse quantization. The peak width Γ_B can be estimated from the condition $\tau^{-1}(\varepsilon \sim \Gamma_B) \sim \Gamma_B$, and we get:

$$\Gamma_B \sim \left(\frac{n}{\pi}\right)^{2/3}\left(\frac{\lambda}{\pi}\right)^{4/3} \gg \frac{1}{\tau_0}, \quad (3)$$

$$\rho_B^{\max} \sim \frac{1}{e^2 \varepsilon_F}\left(\frac{n}{\pi}\right)^{2/3}\left(\frac{\lambda}{\pi}\right)^{4/3} \gg \rho_0. \quad (4)$$

Let us now take into account single-impurity non-Born effects in scattering. For an impurity placed on the wall of the tube, the renormalized scattering amplitude $\Lambda^{(\text{ren})}$ may be found from Dyson equation. As a result:

$$\lambda \to \Lambda^{(\text{ren})}(\varepsilon) \approx \lambda\left(1 + \frac{\Lambda_{2D}}{\pi\sqrt{-\varepsilon}}\right). \quad (5)$$

$\Lambda_{2D} \approx \lambda - i\lambda^2$ being an exact scattering amplitude on 2D plane. From (5) we see that non-Born effects are essential for $\varepsilon < \varepsilon_{\text{nB}} = (\lambda/\pi)^2 \ll 1$. The questions arises: what happens first upon approaching the singularity: the single-impurity non-Born effects develop, or the singularity is smoothed due to scattering? The answer is given by comparison of Γ_B and ε_{nB}, so we arrive at the following criterion of relevance of single-impurity non-Born effects:

$$n < n_c, \quad n_c = |\lambda|/\pi. \quad (6)$$

Below we summarize the properties of the $\rho(\varepsilon)$ near the singularity in the "non-Born regime". Above the singularity (for $\varepsilon > 0$) the scattering time and the resistivity

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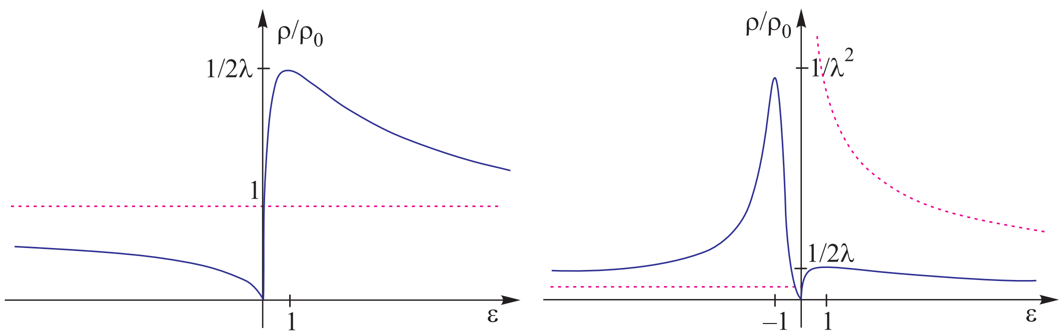

Fig. 1. Non-Born resistivity ρ as a function of chemical potential ε; $\epsilon = \varepsilon/\varepsilon_{\rm nB}$. Left: repulsing impurities ($\lambda > 0$). Right: attracting impurities ($\lambda < 0$)

are not sensitive to the sign of λ and have smooth maximum at $\varepsilon = \varepsilon_{\rm nB}$:

$$\frac{1}{\tau(\varepsilon)} = 2\left(\frac{n}{\pi}\right)\left(\frac{\lambda}{\pi}\right) F\left(\frac{\varepsilon}{\varepsilon_{\rm nB}}\right), \quad F(z) = \frac{1}{z^{1/2}+z^{-1/2}}. \tag{7}$$

Its value at maximum is $\rho_{\rm nB}^{\max(+)} \sim \frac{2}{e^2\varepsilon_F}\left(\frac{n}{\pi}\right)\left(\frac{\lambda}{\pi}\right)^2 \ll \ll \rho_B^{\max}$ is lower, than in the Born case.

Below the singularity (for $\varepsilon < 0$) the result is sensitive to the sign of λ (see Fig. 1).

For repulsing impurities in case $\varepsilon < 0$ we get:

$$\frac{1}{\tau(\varepsilon)} = 2\pi\left(\frac{n}{\pi}\right)\left(\frac{\lambda}{\pi}\right)^2 \tilde{F}_{\rm rep}\left(\frac{\varepsilon}{\varepsilon_{\rm nB}}\right), \tag{8}$$

$$\tilde{F}_{\rm rep}(z) = \left(1+(-z)^{-1/2}\right)^{-2}. \tag{9}$$

For attracting impurities the scattering amplitude $\Lambda^{(\rm ren)}(\varepsilon)$ has a pole at $\varepsilon = (-1+2i|\lambda|)\varepsilon_{\rm nB}$ and for $|\lambda| \ll 1$ it is close to real axis which results in a resonant peak of the resistivity. Physically, this pole emerges as a manifestation of a quasi-stationary state that arises under the bottom of each subband due to attractive potential (whatever small!). Indeed, the density of states in resonant subband is huge compared to other subbands and therefore an electron spends almost all time in this subband. In other words, it is effectively almost one-dimensional one, and we know that in 1D case an arbitrary weak attracting potential inevitably forms a bound state. If we, however, take into account rare transitions to non-resonant subbands, then this bound state acquires finite lifetime and the resistivity peak acquires finite width $\Gamma_{\rm nB}^{(-)} = 4|\lambda|\varepsilon_{\rm nB}$. The shape of resistivity is described by formula (9) with the substitution $\tilde{F}_{\rm rep} \to \tilde{F}_{\rm attr}$:

$$\tilde{F}_{\rm attr}(z) \approx \begin{cases} (1-|z|^{-1/2})^{-2}, & |1-|z|| \gg |\lambda|, \\ \frac{4}{(1-|z|)^2+4\lambda^2}, & |1-|z|| \lesssim |\lambda|. \end{cases} \tag{10}$$

Resistivity maximum $\rho_{\rm nB}^{\max(-)} \sim \frac{1}{e^2\varepsilon_F}\frac{2n}{\pi^2}$ with a width $\Gamma_{\rm nB}^{(-)}$ is attained at $\varepsilon = -\varepsilon_{\rm nB}$.

One of the most striking features of the obtained results is vanishing of the resistivity at $\varepsilon \to 0$, as a consequence of the suppression of $\Lambda^{(\rm ren)}$ for $\varepsilon \to 0$. This zero in resistivity is, indeed, an artefact of the single impurity approximation: the resistivity actually vanishes only in the linear in n approximation. Upon taking into account scattering at other impurities, we get not an exact zero, but some minimum resistivity $\rho_{\min} \propto n^3$ attained at $\varepsilon \sim -n^2$.

Comparing the above results with the formula (1) we see that

(i) The Fano theory is not able to reproduce the curve of the "plateau minimum-maximum-plateau" type, characteristic for the case of attracting impurities.

(ii) The curve of the "plateau-maximum-plateau" type, in principle, can be generated by the Fano formula, but the structure of this type can be expected only in case of repulsion, when there is no resonant states and, therefore, no reason to invoke the Fano resonances.

The present theory, explains complex structures of the Van Hove singularities in quasi-one-dimensional systems as being due to non-Born effects in scattering. Predictions of this theory can be easily discriminated from those of the Fano theory.

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