Non-Born effects in scattering of electrons in weakly disordered quasi-1D systems

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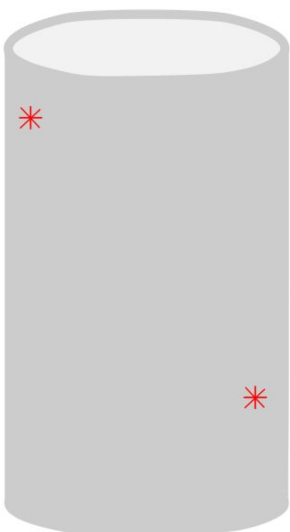
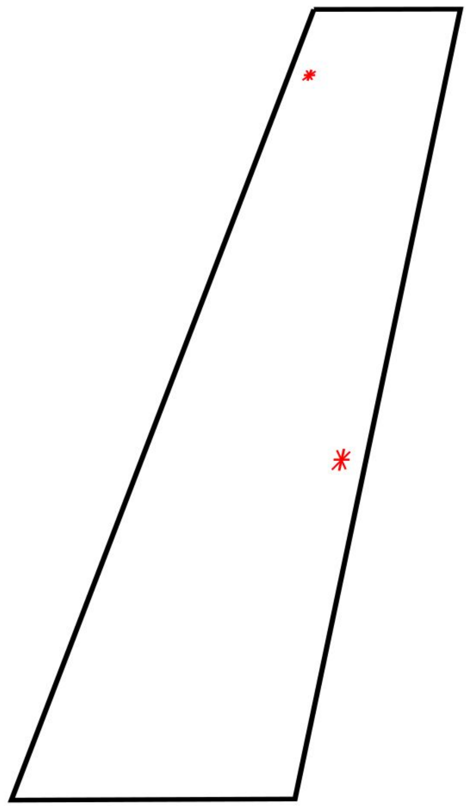
[1] A. S. Ioselevich, N. S. Peshcherenko, Phys. Rev. B 99, 035414 (2019); arXiv:1810.00426.

[2] A. S. Ioselevich, N. S. Peshcherenko, Письма в ЖЭТФ, 108(12), 825-826 (2018)

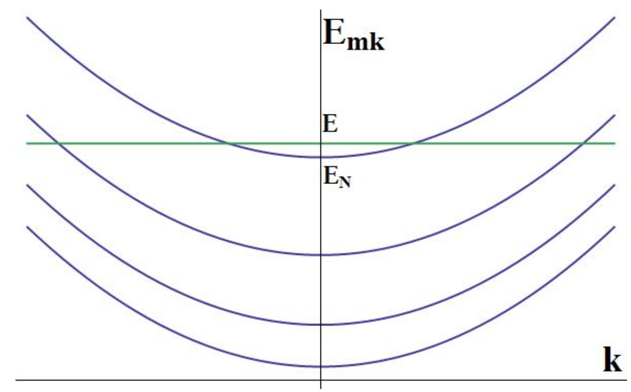
Quasi-1D systems: examples



Carbon nanotubes



2D gated nanoconstrictions



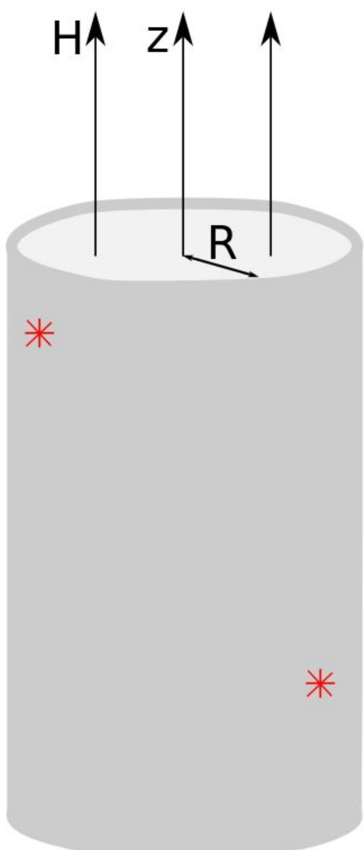
Quasi-1D = 1D subbands of transversal quantization

Principal assumptions

- Clean case: $l(\varepsilon) \gg R$, $l(\varepsilon)$ - mean free path, R - transversal size. However, $l(\varepsilon) \ll L$, L - system length
- Weak scattering: $|\lambda| \ll 1$, λ - dimensionless scattering amplitude
- Semiclassical case: $\lambda_F \ll R$ and $L \ll L_{loc}$

Problem statement

- Strip and a tube in longitudinal magnetic field
- Ideally clean case - square root Van Hove singularities
- How Van Hove singularities are smeared due to scattering (beyond Born approximation as well)?

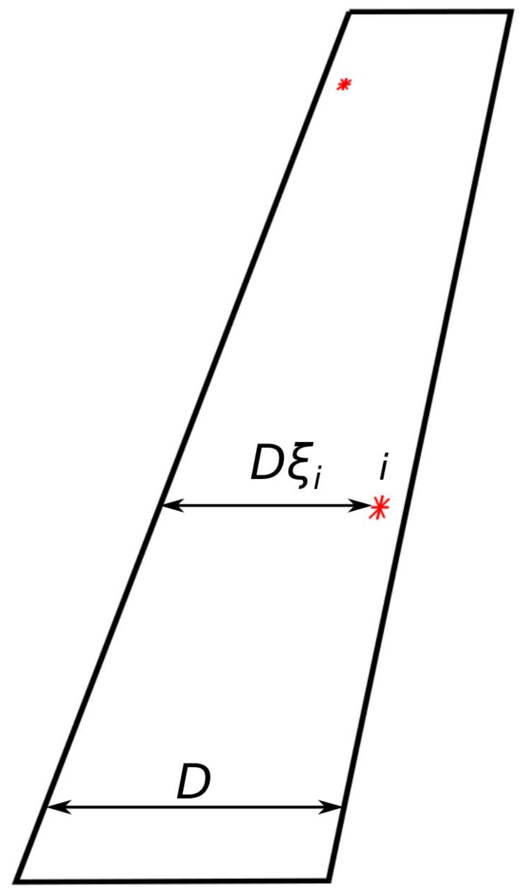


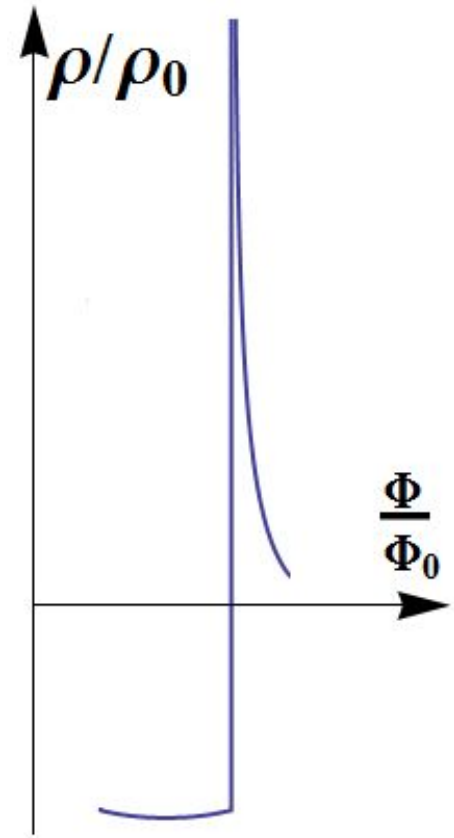
Magnetic flux

$$\Phi = \pi R^2 H$$

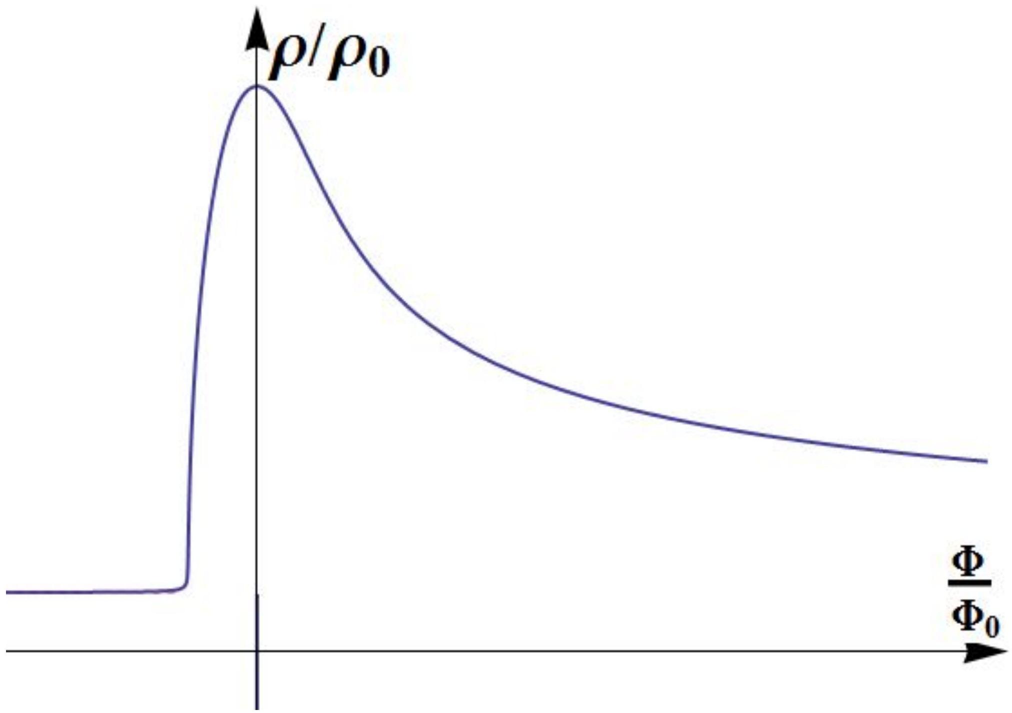
Flux quantum

$$\Phi_0 = \frac{\pi \hbar c}{e}$$



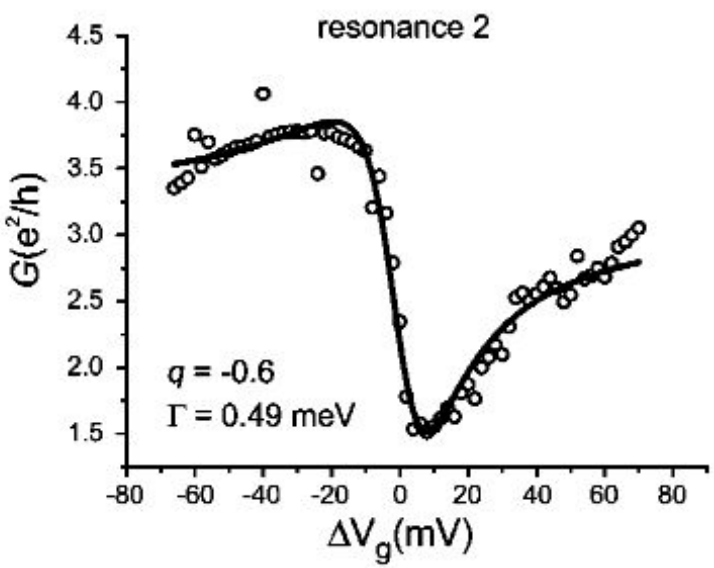


Trivial scenario: smoothing of singularity



[1] H. L. Frish, S. P. Lloyd, Phys. Rev., 120, 1179 (1960)
[2] S. Hügle, R. Egger, Phys. Rev. B 66, 193311 (2002)
[3] I.M.Lifshitz, S.A.Gredeskul, and L.A.Pastur, Introduction to the Theory of Disordered Systems. Science, Moscow, (1982).

Experiment: more complex scenarios



Phenomenologically these results were attributed to Fano resonances

[1] B. Babić and C. Schönenberger, Phys. Rev. B 70, 195408 (2004)
[2] Z. Zhang, D. A. Dikin, R. S. Ruo, and V. Chandrasekhar, Europhysics Letters, 68, 713 (2004)

$$\rho(E) \propto \frac{\left(E - E_N + q\Gamma/2\right)^2}{\left(E - E_N\right)^2 + \left(\Gamma/2\right)^2}$$

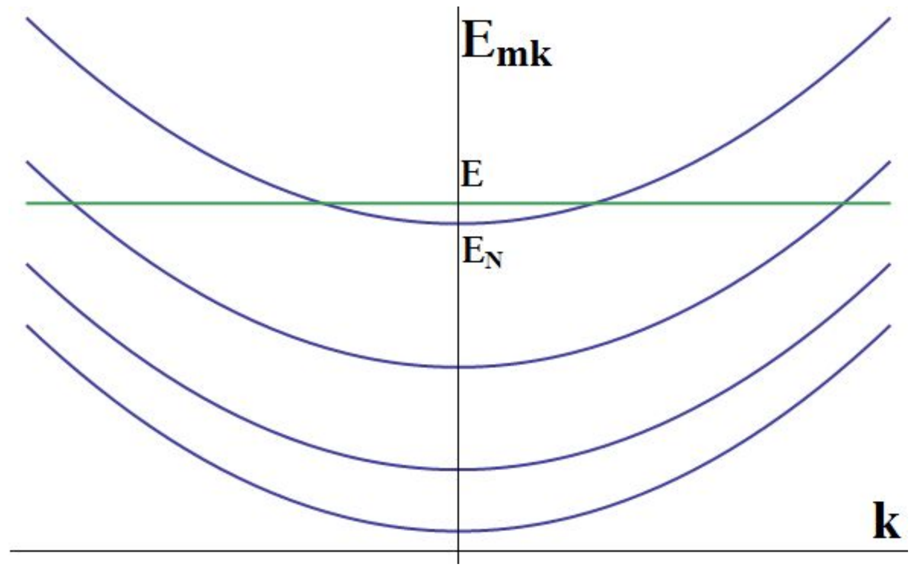
However, we show that similar curve could be simply a consequence of non-Born scattering.

Outline

- Smearing of Van Hove singularities within Born approximation
- Applicability criterion for Born approximation. Requirement for relatively high impurity concentration $n > |\lambda|/\pi$
- Origin of non-Born effects. Criterion of non-Born regime:
$$n < |\lambda|/\pi$$
- Single impurity scattering approximation within resonant subband
- Quasistationary states
- Multi-impurity effects
- Conclusions

Ideal system

- Spectrum: set of 1D subands: $E_{mk} = E_0\left(m + \Phi/2\Phi_0\right)^2 + \dfrac{k^2}{2m^*}, \quad E_0 = \dfrac{1}{2m^* R^2} \qquad m \in \mathbb{Z}$
- Units of length $2\pi R, D,$
- Units of energy E_0



$$E - E_N = \varepsilon E_0$$

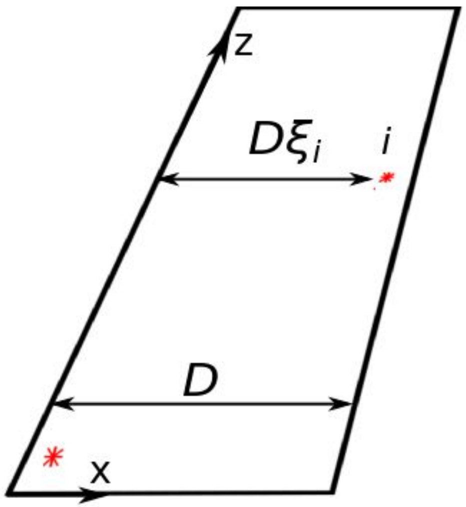
- Density of states

$$\nu(\varepsilon) = \sum_{m=-\infty}^{\infty} \nu_m(\varepsilon) = \sum_{m=-\infty}^{\infty} \frac{\theta(\varepsilon_m)}{\sqrt{\varepsilon_m}} \approx \nu_0\left(1 + \frac{\theta(\varepsilon_N)}{\pi\sqrt{\varepsilon_N}}\right)$$

Born approximation: tube

- Hamiltonian (point-like impurities) $H = H_{kin} + V\sum_i \delta(\mathbf{r} - \mathbf{r}_i)$
- Matrix elements: $V^{(i)}_{kk'mm'}(\phi_i, z_i) = \dfrac{V}{2\pi R} \exp\{i(k-k')z_i + i(m-m')\phi_i\}$
- All impurities are equivalent: $|V^{(i)}_{kk'mm'}(\phi_i, z_i)|^2$ depends neither on z_i, nor on ϕ_i

Born approximation: strip



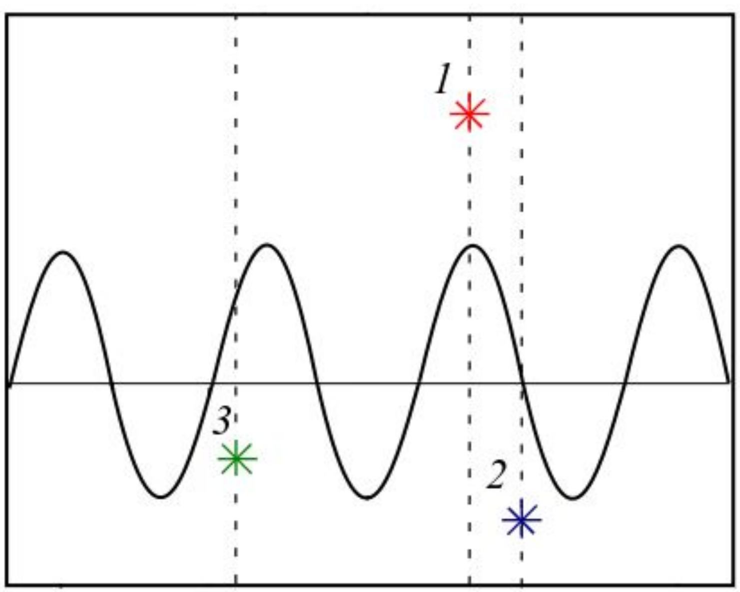
- Hamiltonian (point-like impurities)

$$H = H_{kin} + V\sum_i \delta(\mathbf{r} - \mathbf{r}_i)$$

- Matrix elements:

$$V^{(i)}_{kk'mm'}(\xi_i, z_i) = \frac{2V}{D}\exp\{i(k-k')z_i\} \times \sin(\pi(m+1)\xi_i)\sin(\pi(m'+1)\xi_i),$$

'Strength' of impurities depends on their position:



'Typical' $\sin^2(\pi(m+1)\xi_i) \sim 1$

strong impurities $\sin^2(\pi(m+1)\xi_i) \approx 1$

weak impurities $\sin^2(\pi(m+1)\xi_i) \approx 0$

Born approximation (away from singularity)

- Density of states: $\nu_0 = \pi$
- Scattering rate: $\tau_0^{-1} = 2n\left(\lambda/\pi\right)^2$
- $\lambda = m^* V/2 \ll 1$ - Born scattering amplitude
- $n \equiv \begin{cases} n_2(2\pi R)^2, & \text{for cylinder,} \\ n_2 D^2, & \text{for strip,} \end{cases}$ $n \ll 1$

Born approximation (near the singularity)

- Scattering rates:

tube

$$\frac{\tau_0}{\tau(\varepsilon)} \approx 1 + \frac{\theta(\varepsilon)}{\pi\sqrt{\varepsilon}}$$

strip

$$\frac{\tau_0}{\tau_m(\varepsilon)} \approx \begin{cases} 1 + \dfrac{\theta(\varepsilon)}{\pi\sqrt{\varepsilon}}, & m \neq N \\ 1 + \dfrac{3\theta(\varepsilon)}{2\pi\sqrt{\varepsilon}}, & m = N \end{cases}$$

Resistivity

- Kubo formula in the Drude approximation

$$\sigma = \frac{e^2}{2\pi}\mathrm{Tr}[\hat{v}_z \hat{G}^R \hat{v}_z \hat{G}^A] = \frac{e^2}{2\pi}\int \frac{dk}{2\pi}\sum_m \frac{(v_{km}^z)^2}{(\varepsilon - E_{km})^2 + 1/4\tau_m^2(\varepsilon)} \approx e^2 \int \frac{dk}{2\pi}\sum_m (v_{km}^z)^2 \delta(\varepsilon - E_{km})\tau_m(\varepsilon)$$

- For resistivity we get: $\dfrac{\rho(\varepsilon)}{\rho_0} = \dfrac{\tau_0}{\tau_{\mathrm{nonres}}(\varepsilon)}$

- Born approximation: $\dfrac{\rho(\varepsilon)}{\rho_0} = \dfrac{\nu(\varepsilon)}{\nu_0}$

Smearing of Van Hove singularities: Born approximation

- Perturbation theory holds for $\tau^{-1}(\varepsilon) \ll \varepsilon$
- For $\varepsilon > 0$ we get the smearing scale $\varepsilon_{\min}$ from the condition:

$$\frac{1}{\tau(\varepsilon)} = \frac{1}{\tau_0}\frac{\nu(\varepsilon)}{\nu_0} = \frac{1}{\tau_0 \pi \sqrt{\varepsilon}} \sim \varepsilon, \quad \Rightarrow \quad \varepsilon_{\min} = (2\pi\tau_0)^{-2/3} \sim \lambda^{4/3} n^{2/3}, \qquad \frac{\rho_{\max}}{\rho_0} \sim \lambda^{-2/3} n^{-1/3}$$

- For $|\varepsilon| \lesssim \varepsilon_{\min}$ we will map some strictly 1D result to our quasi-1D problem

Strictly 1D system: exact results

Valid only for

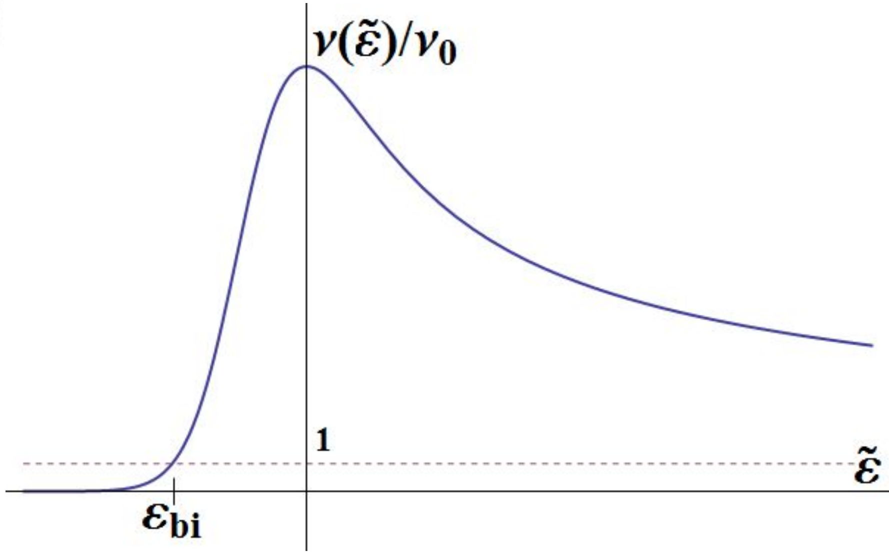
$$n \gg |\lambda|$$

- Density of states: $\nu_{\mathrm{res}}^{(\mathrm{t})}(\tilde{\varepsilon}) = \nu_0 \left(\tilde{\varepsilon}_{\mathrm{min}}^{(\mathrm{t})}\right)^{-1/2} Y\left(\tilde{\varepsilon}/\tilde{\varepsilon}_{\mathrm{min}}^{(\mathrm{t})}\right)$ $\quad \tilde{\varepsilon}_{\mathrm{min}}^{(\mathrm{t})} = (2\pi\tau_0)^{-2/3}$

- Average potential: $\overline{U} = \left\langle V \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle_{\mathbf{r}_i} = \dfrac{\lambda n}{\pi^2}$ $\quad \tilde{\varepsilon} = \varepsilon - \overline{U}$

$$Y(q) = \frac{2}{\sqrt{\pi}} \frac{\partial}{\partial q} \left(\int_0^\infty \frac{dx}{\sqrt{x}} \exp\left\{ -xq - \frac{x^3}{12} \right\} \right)^{-1}$$

$$Y(q) \approx \begin{cases} \frac{1}{\pi\sqrt{q}}, & q > 0, \quad q \gg 1 \\ |q| \exp\left(-\frac{4}{3}|q|^{3/2}\right), & q < 0, \quad |q| \gg 1. \end{cases}$$



Random potential is effectively gaussian

H. L. Frish, S. P. Lloyd, Phys. Rev., 1960, 120, p 1179

Density of states: from 1D to quasi-1D

- $\nu(\tilde{\varepsilon}) \approx \nu_{\text{nonres}}(\tilde{\varepsilon}) + \nu_{\text{res}}(\tilde{\varepsilon})$
- Bifurcation point $\tilde{\varepsilon}_{\text{bi}}^{(\text{t})}$: is defined by $\nu_{\text{nonres}}^{(\text{t})}(\tilde{\varepsilon}_{\text{bi}}^{(\text{t})}) = \nu_{\text{res}}^{(\text{t})}(\tilde{\varepsilon}_{\text{bi}}^{(\text{t})})$. As a result:

$$\varepsilon_{\text{bi}}^{(\text{t})} \approx -(3/8)^{2/3}\,\varepsilon_{\text{min}}^{(\text{t})} \ln^{2/3}\left(1/\tilde{\varepsilon}_{\text{min}}^{(\text{t})}\right)$$

- Hybridization between resonant and nonresonant states gives only a small correction to the density of states:

$$\delta\nu(\varepsilon) \propto -\nu_0 n \lambda^2 \frac{d}{d\varepsilon}\int \frac{\nu(\varepsilon')d\varepsilon'}{\varepsilon-\varepsilon'} \propto \nu_0 \left(\frac{\varepsilon_{\text{min}}}{|\varepsilon|}\right)^{3/2} \propto \frac{\nu_0}{\ln\left(\varepsilon_{\text{min}}^{-1}\right)} \ll \nu_0$$

for $\varepsilon = \varepsilon_{\text{bi}}^{(\text{t})}$

- Thus,

$$\frac{\nu^{(\text{t})}(\tilde{\varepsilon})}{\nu_0} = \frac{\rho^{(\text{t})}(\tilde{\varepsilon})}{\rho_0} \approx 1 + \left(\tilde{\varepsilon}_{\text{min}}^{(t)}\right)^{-1/2} Y\left(\tilde{\varepsilon}/\tilde{\varepsilon}_{\text{min}}^{(\text{t})}\right)$$

Role of the resonant subband

- Resonant subband states do not contribute to current directly!

- The resonant subband affects the resistivity only through the density of final states for scattering of current carrying nonresonant states

- Although we calculate the resistivity of the system, from the resonant subband we need only the density of states.

Origin of non-Born effects

- Perturbative matrix elements (all processes within resonant subband are taken into account nonperturbatively)

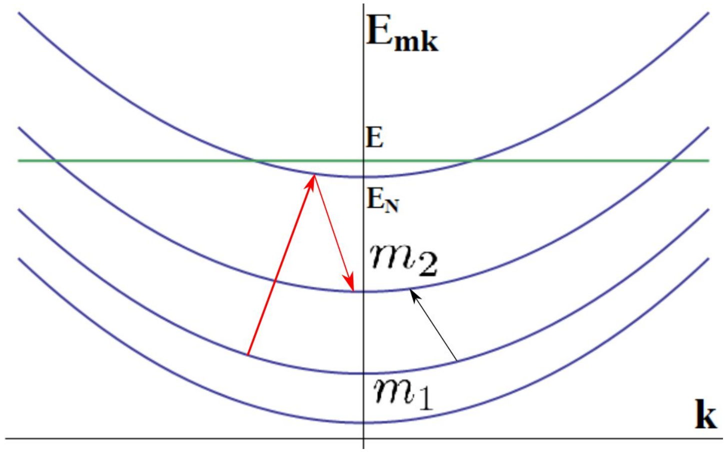
$$\tilde{V}^{(i)}_{m_1,m_2} = V^{(i)}_{m_1,m_2} + V^{(i)}_{m_1,N} G^{(\mathrm{res})}_{\varepsilon}(z_i, z_i) V^{(i)}_{N,m_2} = \\ = \frac{\tilde{\lambda}_i}{\pi^2} \chi_{m_1}(\mathbf{r}_i) \chi^*_{m_2}(\mathbf{r}_i),$$

$$\chi_m(\mathbf{r}_i) = \\ \begin{cases} \exp\{m\phi_i\}, & (\mathrm{tube}), \\ \sqrt{2}\sin(\pi m \xi_i), & (\mathrm{strip}). \end{cases}$$

- Multiple scattering (with necessary excursions to the resonant subband)

$$\tilde{V}^{(i)(\mathrm{ren})}_{m_1,m_2} = \tilde{V}^{(i)}_{m_1,m_2} + \sum_{m \neq N} \tilde{V}^{(i)}_{m_1,m} g^{(m)}_{\varepsilon}(0) \tilde{V}^{(i)}_{m,m_2} + \\ + \sum_{m,m' \neq N} \tilde{V}^{(i)}_{m_1,m} g^{(m)}_{\varepsilon}(0) \tilde{V}^{(i)}_{m,m'} g^{(m')}_{\varepsilon}(0) \tilde{V}^{(i)}_{m',m_2} + \ldots,$$

$$g^{(m)}_{\varepsilon}(0) = \int \frac{dk}{2\pi} \left\{ \varepsilon_m - \frac{k^2}{(2\pi)^2} + i0 \right\}^{-1} = -\frac{\pi i}{\sqrt{\varepsilon_m}}$$



black line - direct transition, red line - composite transition with an excursion to resonant subband

Scattering amplitude

- Summing up perturbation series, one could obtain scattering amplitude:

$$\tilde{\Lambda}_i^{(\mathrm{ren})} = \Lambda \left\{ 1 + \frac{\Lambda_i}{\pi^2 Q_i + \Lambda_i^*} \right\}, \qquad \tilde{V}_{m_1,m_2}^{(i)(\mathrm{ren})} = \frac{\tilde{\Lambda}_i^{(\mathrm{ren})}}{\pi^2} \chi_{m_1}(\mathbf{r}_i) \chi_{m_2}^*(\mathbf{r}_i)$$

$$Q_i = \left[G_\varepsilon^{(\mathrm{res})}(z_i, z_i) \right]^{-1} - \lambda_i/\pi^2, \qquad \lambda_i \equiv \lambda |\chi_N(\mathbf{r}_i)|^2 \quad \Lambda_i = \Lambda |\chi_N(\mathbf{r}_i)|^2$$

Λ - exact 2D scattering amplitude

- Since $\Sigma_m^{(i)} = \tilde{V}_{m,m}^{(i)(\mathrm{ren})}$, we obtain scattering rate:

$$\tau_{mk}^{-1} = -\frac{2}{\pi^2} \sum_i |\chi_m(\mathbf{r}_i)|^2 \mathrm{Im} \left\{ \tilde{\Lambda}_i^{(\mathrm{ren})} \right\} = -\frac{2n}{\pi^2} \int_0^1 d\xi |\chi_m(\xi)|^2 \mathrm{Im} \left\{ \tilde{\Lambda}^{(\mathrm{ren})}(\xi, \varepsilon) \right\}$$

Finding $G_\varepsilon^{(\mathrm{res})}(z_i, z_i)$

- Green function satisfies the following equation:

$$\left\{-\frac{d^2}{(2\pi)^2 dz^2} + \sum_i \frac{\lambda_i}{\pi^2}\delta(z - z_i) - \varepsilon\right\} G_\varepsilon^{(\mathrm{res})}(z) = -\delta(z)$$

- For not very low ε single impurity approximation is sufficient:

$$\left\{-\frac{d^2}{(2\pi)^2 dz^2} + \frac{\lambda_i}{\pi^2}\delta(z) - \varepsilon\right\} G_\varepsilon^{(\mathrm{res})}(z) = -\delta(z) \qquad G_\varepsilon^{(\mathrm{res})}(0,0) = \frac{\pi}{i\sqrt{\varepsilon} - \lambda_i/\pi}$$

- Finally, scattering amplitude is

$$\epsilon_i \equiv \epsilon |\chi_N(\mathbf{r}_i)|^{-4},$$

$$\tilde{\Lambda}_i^{(\mathrm{ren})} = \frac{i\sqrt{\epsilon_i}|\lambda|(1 - i\lambda)}{i\sqrt{\epsilon_i}\mathrm{sign}\lambda - (1 - i\lambda)}$$

$$\epsilon = \frac{\varepsilon}{\varepsilon_{\mathrm{nB}}}, \quad \varepsilon_{\mathrm{nB}} \equiv \left(\frac{\lambda}{\pi}\right)^2$$

Non-Born regime criterion

- $$\tilde{\Lambda}_i^{(\mathrm{ren})} = \frac{i\sqrt{\epsilon_i}|\lambda|(1-i\lambda)}{i\sqrt{\epsilon_i}\mathrm{sign}\lambda - (1-i\lambda)}$$

$$\epsilon_i \equiv \epsilon|\chi_N(\mathbf{r}_i)|^{-4},$$

$$\epsilon = \frac{\varepsilon}{\varepsilon_{\mathrm{nB}}}, \quad \varepsilon_{\mathrm{nB}} \equiv \left(\frac{\lambda}{\pi}\right)^2$$

- $\tilde{\Lambda}^{(\mathrm{ren})} \to 0$ for $\epsilon_i \to 0$, thus non-Born effects are most spectacular for

$$\varepsilon \ll \varepsilon_{\mathrm{nB}}$$

- Comparing $\varepsilon_{\mathrm{nB}}$ and $\tilde{\varepsilon}_{\min}$, we arrive at the following criterion of non-Born regime:

$$\tilde{\varepsilon}_{\min} < \varepsilon_{\mathrm{nB}}, \quad \text{or} \quad n < n_c = |\lambda|/\pi$$

Non-Born case.
$\rho(\varepsilon)$: repulsing impurities $(\lambda > 0)$

- Thus, for $\rho(\varepsilon)$ we get:

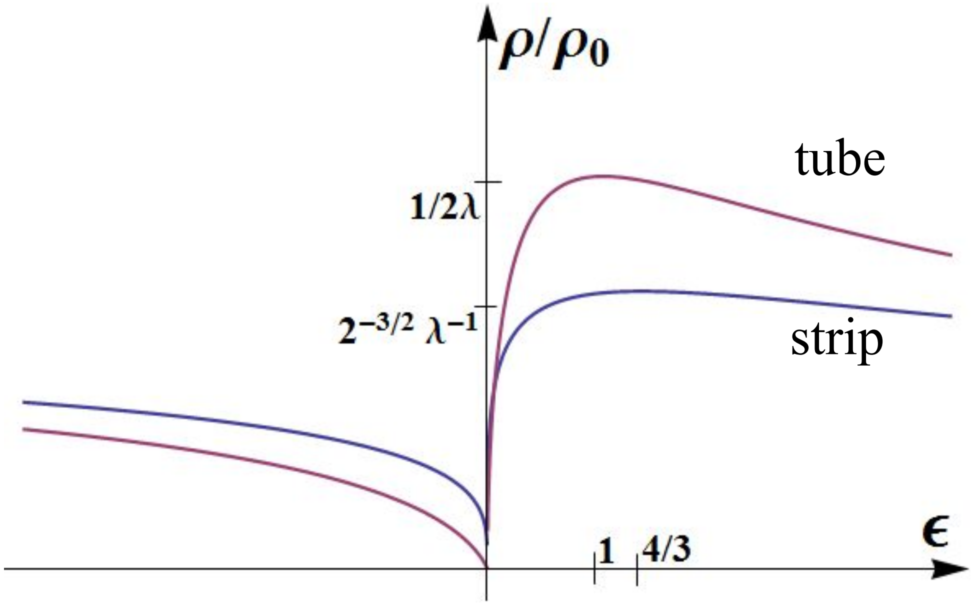
For $\varepsilon > 0$

$$\frac{\rho(\epsilon)}{\rho_0} \approx \begin{cases} \dfrac{\epsilon^{1/2}}{\lambda}, & \text{for cylinder} \\ \dfrac{\epsilon^{1/4}}{2\lambda}, & \text{for strip} \end{cases}, \quad \epsilon \ll 1$$

For $\varepsilon < 0$

$$\frac{\rho(\epsilon)}{\rho_0} \approx \begin{cases} |\epsilon|, & \text{for cylinder} \\ \dfrac{|\epsilon|^{1/4}}{2\sqrt{2}}, & \text{for strip} \end{cases}, \quad |\epsilon| \ll 1$$

- Here $\epsilon = \varepsilon / \varepsilon_{\rm nB}$

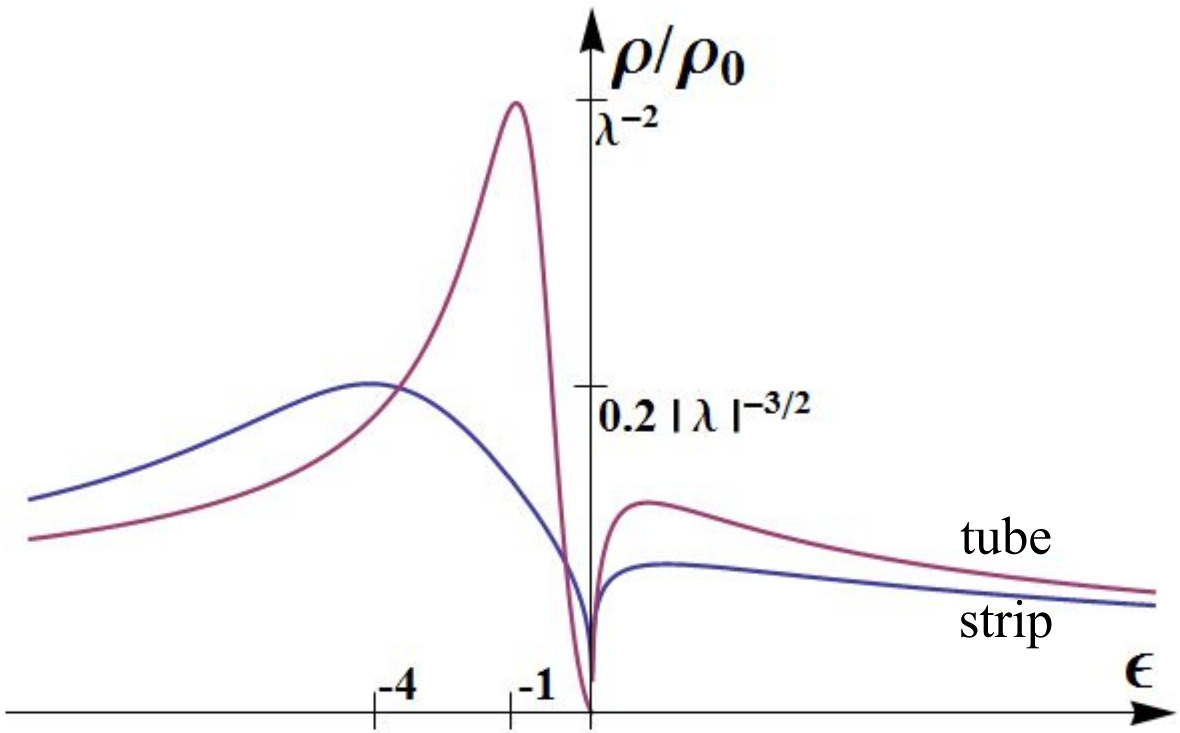


Strip: since scattering amplitude depends on the position of impurity, maximum is somewhat broadened

Non-Born case.
$\rho(\varepsilon)$: attractive impurities $(\lambda < 0)$

- For $\varepsilon > 0$ $\rho(\varepsilon)$ does not depend on the sign of λ
- For $\varepsilon < 0$ - scattering amplitude has a pole at $\varepsilon = (-1 + 2i|\lambda|)(\lambda_i/\pi)^4$
- $$\frac{\rho(\epsilon)}{\rho_0} \approx \begin{cases} |\epsilon|, & \text{for cylinder} \\ \dfrac{|\epsilon|^{1/4}}{\lambda}, & \text{for strip} \end{cases}, \quad |\epsilon| \ll 1$$

Left peak is due to quasistationary states.



Non-Born case (quasistationary states)

- Quasistationary states (poles of scattering amplitude):

tube

$$\epsilon_{\text{qs}} = (-1 + 2i|\lambda|)$$

strip

$$\epsilon_{\text{qs}} = 4\sin^4(\pi N \xi_i)(-1 + 2i|\lambda|)$$

- Finite width due to transitions to nonresonant subbands
- Tube case: the same ϵ_{qs} for all impurities. However, not the case for strip.

Quasistationary states (strip case)

- $\epsilon_{\mathrm{qs}} = 4\sin^4(\pi N\xi_i)(-1+2i|\lambda|)$
- Impurity band: $-4 < \epsilon_{\mathrm{qs}} < 0$. Distribution function for energies (strip):

$$P(\varepsilon_{\mathrm{qs}}) = \frac{\theta(-\epsilon_{\mathrm{qs}})\theta(\epsilon_{\mathrm{qs}}+4)}{2\pi}\frac{2+\sqrt{|\epsilon|}}{\sqrt{|\epsilon|_{\mathrm{qs}}^{3/2}(4-|\epsilon_{\mathrm{qs}}|)}}$$

different $\rho(\varepsilon \to -0)$ than for tube

- 'Van-Hove like' singularity near the edge of the impurity band:

$$\frac{\rho(\epsilon)}{\rho_0} = \begin{cases} 8\sqrt{2}\,(|\epsilon|-4)^{-3/2}, & \text{for } 4+\epsilon \to -0, \\ \frac{2\sqrt{2}}{|\lambda|}(4-|\epsilon|)^{-1/2}, & \text{for } 4+\epsilon \to +0. \end{cases}$$

smeared at $|\epsilon+4| \lesssim |\lambda|$

- For $-4 < \epsilon < 0$ scattering predominantly happens at resonant impurities $\epsilon = \epsilon_{\mathrm{qs}}(\xi_i)$
- Scattering for $\epsilon \to -4$ - predominantly at strong impurities, for $\epsilon \to 0$ at weak impurities

Multi-impurity effects

- Multi-impurity effects are negligible for $\tau_{\mathrm{res}}^{-1}(\varepsilon) < \varepsilon$ and essential for

$$\varepsilon < \varepsilon_{\mathrm{min}}^{\mathrm{nB}}$$

where $\varepsilon_{\mathrm{min}}^{\mathrm{nB}}$ is determined by

$$\tau_{\mathrm{res}}^{-1}(\varepsilon_{\mathrm{min}}^{\mathrm{nB}}) \sim \varepsilon_{\mathrm{min}}^{\mathrm{nB}}, \Rightarrow \varepsilon_{\mathrm{min}}^{\mathrm{nB}} \sim n^2$$

- Since $\tau^{-1}(\varepsilon \to 0) \to 0$, one should expect some minimum of $\rho(\varepsilon)$ at

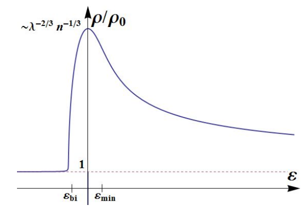
$$|\varepsilon| \lesssim \varepsilon_{\mathrm{min}}^{\mathrm{nB}}$$

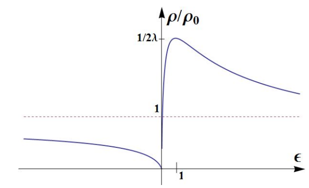
Conclusions

2 distinct regimes with respect to concentration:

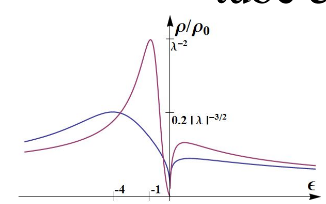
- Born regime $(n \gg n_c)$- singularity structure is 'plateau-maximum-plateau'
- Non-Born regime $(n \ll n_c)$
  - Repulsing impurities:
  'plateau-minimum-maximum-plateau'
  - Attractive impurities: 'plateau-maximum-minimum-maximum-plateau', quasistationary states are important.
- Strip case: quasistationary states form impurity band $-4 < \epsilon < 0$, in which resonant scattering determines $\rho(\varepsilon)$
- Minimum of $\rho(\varepsilon)$ near the Van Hove singularity (at the energies of the order of $\sim n^2$) is expected

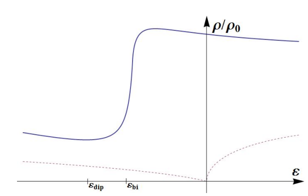
tube & strip





tube & strip





tube