Non-Born effects in resistivity of quasi-1D systems

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Quasi-1D-Systems: Examples



Assumed: Weak short-range impurities sitting at the surface at low concentration

Spectrum of clean Quasi-1D-System:



Spectrum consists of a series of 1D subbands

Parameters

- L length of the sample, R transverse size, p_F Fermi momentum
- $N \sim p_F R$ number of available channels
- λ dimensionless scattering amplitude
- n_2 2D concentration of impurities
- $l(\varepsilon)$ mean free path
- $L_{\rm loc} \sim Nl(\varepsilon)$ localization length

Conditions





What are we going to study?

Ideally clean case: square root Van Hove singularities (when Fermi level crosses a bottom of some subband)



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

Flux quantum $\Phi_0 = \frac{\pi \hbar c}{e}$ Dirty case: only first harmonic survives



What happens with singularities in clean (but not ideal) case?

Trivial scenario: smoothing of singularity



Strictly 1D case, Born approximation

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

Experiment: more complex scenarios



- B. Babić and C. Schönenberger, Phys. Rev. B 70, 195408 (2004)
- Z. Zhang, D. A. Dikin, R. S. Ruo, and V. Chandrasekhar, Europhys. Letters, **68**, 713 (2004)

Phenomenologically these results were attributed to Fano resonances

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

Fano resonance: single-band scattering at quasidiscrete (attracting) level We show:

- Multiband structure is essential, Non-Born effects are essential;
- Resonance-like behavior possible without quasidiscrete states (e. g., for repulsion)

Outline

- Smearing of Van Hove singularities within Born approximation
- Applicability criterion for Born approximation. Requirement for relatively high impurity concentration: $n > n_c \sim |\lambda|$
- NonBorn effects: strong renormalization of scattering amplitude for low impurity concentration $n < n_c$
- Attracting impurities ($\lambda < 0$): quasistationary states
- Peculiarities of the strip case
- Discussion

Ideal system



• Density of states

$$\boldsymbol{\nu}(\varepsilon) = \sum_{m=-\infty}^{\infty} \boldsymbol{\nu}_{m}(\varepsilon) = \sum_{m=-\infty}^{\infty} \frac{\theta(\varepsilon_{m})}{\sqrt{\varepsilon_{m}}} \approx \boldsymbol{\nu}_{0} \left(1 + \frac{\theta(\varepsilon_{N})}{\pi\sqrt{\varepsilon_{N}}}\right)$$

• Semiclassical density of states $v_0 = \pi$

Born approximation: Tube

Hamiltonian (point-like impurities)

$$H = H_{kin} + V \sum_{i} \delta \left(\mathbf{r} - \mathbf{r}_{i} \right)$$

Matrix elements:

$$V_{kk'mm'}^{(i)}(\phi_i, z_i) = \frac{V}{2\pi R} \exp\{i(k - k')z_i + i(m - m')\phi_i\}$$

All impurities are equivalent:

$$|V_{kk'mm'}^{(i)}(\phi_i,z_i)|^2$$
 depends neither on z_i , no on ϕ_i



Born approximation: Strip

Hamiltonian (point-like impurities)

$$H = H_{kin} + V \sum_{i} \delta \left(\mathbf{r} - \mathbf{r}_{i} \right)$$

Matrix elements:



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

"Strength" of impurities depends on their position:

• "Typical" impurities: $\sin^2(\pi(m+1)\xi_i) \sim 1$

• 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: $\nu_0 = \pi$

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Scattering rate:
$$\frac{1}{\tau_{mk}} \equiv \frac{1}{\tau_0} = 2\pi \left(\frac{\lambda}{\pi}\right)^2$$

• Born scattering amplitude $\lambda = m^* V / 2 \ll 1$

$$n \equiv \begin{cases} n_2 (2\pi R)^2, & \text{for cylinder,} \\ n_2 D^2, & \text{for strip,} \end{cases} \qquad n \ll 1$$

Born approximation (near the singularity)

Scattering rates:



Resistivity

• Kubo formula (in the Drude approximation):

$$\sigma_{zz} = \frac{e^2}{2\pi} \operatorname{Tr} \left[\mathbf{v}_z G^R \mathbf{v}_z G^A \right] = \frac{e^2}{2\pi} \sum_{\alpha} \mathbf{v}_{z\alpha}^2 \frac{1}{\left(\varepsilon - \varepsilon_{\alpha} \right)^2 + 1/4\tau^2} = e^2 D v_{tr}$$

• Diffusion coefficient $D = \mathbf{v}_F^2 \tau/2$

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- "Transport density of states" $v_{tr}(\varepsilon) = 2\sum_{\alpha} \left(\frac{\mathbf{v}_{z\alpha}}{\mathbf{v}_{F}}\right)^{2} \delta(\varepsilon - \varepsilon_{\alpha})$ Standard density of states $v(\varepsilon) = \sum_{\alpha} \delta(\varepsilon - \varepsilon_{\alpha})$
- The transport density, in contrast to the standard one, does not have singularities!

So that
$$v_{tr}(\varepsilon) = 2 \int \frac{dk}{2\pi} \left(\frac{k}{p_F}\right)^2 \sum_{m} \delta\left(\varepsilon - E_m - \frac{k^2}{2m^*}\right) \propto \sum_{m} \sqrt{\varepsilon_m} \theta(\varepsilon_m)$$
$$\left(v_{tr}(\varepsilon_F) - v_0\right) / v_0 = 1 + O\left(\varepsilon_0^{-3/4}\right)$$

$$\frac{\rho}{\rho_0} = \frac{D_0 v_{tr}}{D v_{tr}} = \frac{\tau_0}{\tau(\varepsilon)} = \frac{v(\varepsilon)}{v_0}, \ \rho_0 = \frac{1}{e^2 \varepsilon_0 \tau_0}$$
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Smearing of Van Hove singularities: Born approximation

- The perturbation theory holds for $|\tau^{-1}(\varepsilon) \ll \varepsilon|$
- Then, for $\varepsilon > 0$ we get the smearing scale ε_{\min} from the condition:

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

• For $\varepsilon < 0$ - the standard perturbation theory can be applied for finding hybridization between the resonant band and nonresonant one:

$$\nu(\varepsilon) = \int d\varepsilon' \, \nu^{(0)}(\varepsilon') \, \delta\left(\varepsilon - \varepsilon' - \delta\varepsilon(\varepsilon')\right) \approx \nu^{(0)}(\varepsilon) \left[1 + \frac{d\delta\varepsilon(\varepsilon)}{d\varepsilon}\right]$$
$$\delta\varepsilon = 2\pi R n_2 \int_0^\infty d\varepsilon' \nu^{(0)}(\varepsilon') \frac{|V|^2}{\varepsilon - \varepsilon'} \propto \tau_0^{-1} \left(-\varepsilon\right)^{-1/2}$$
$$\delta\nu(\varepsilon) \propto \nu_0 \left(\frac{\varepsilon_{\min}}{|\varepsilon|}\right)^{3/2}$$
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Non-matching asymptotics: indication for bifurcation point

The perturbation theory gives:

Asymptotics at $\varepsilon > 0$ and at $\varepsilon < 0$ do not match!

$$\nu(\varepsilon) - \nu_{0} \sim \nu_{0} \begin{cases} \frac{1}{\pi\sqrt{\varepsilon}}, \varepsilon > 0, \varepsilon_{\min} \ll \varepsilon \ll 1\\ \left(\frac{\varepsilon_{\min}}{|\varepsilon|}\right)^{3/2}, \varepsilon < 0, \varepsilon_{\min} \ll |\varepsilon| \ll 1 \end{cases}$$



It hints that there should be a bifurcation point ε_{bi} Near this point $\rho(\varepsilon)$ drops dramatically

It could be justified within SCBA, but we will employ a more legitimate approach...

In the vicinity of singularity density of states is dominated by resonant band. Let us first neglect contributions of all others...



Density of states: from1D to quasi-1D

 $\nu(\tilde{\varepsilon}) \approx \nu_{\rm nonres}(\tilde{\varepsilon}) + \nu_{\rm res}(\tilde{\varepsilon})$

Bifurcation point
$$\tilde{\varepsilon}_{bi}^{(t)}$$
 is defined by condition $\nu_{nonres}^{(t)}(\tilde{\varepsilon}_{bi}^{(t)}) = \nu_{res}^{(t)}(\tilde{\varepsilon}_{bi}^{(t)}).$
As a result
 $\varepsilon_{bi}^{(t)} \approx -(3/8)^{2/3} \varepsilon_{min}^{(t)} \ln^{2/3} \left(1/\tilde{\varepsilon}_{min}^{(t)}\right)$

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

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

As a result:

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

Role of the resonant band

- States within the resonant band do not contribute to current directly!
- The resonant band affects the resistivity only through the density of final states for scattering of current carrying nonresonant states
- Although we are interested in the resistivity of the system, from the resonant band we need only the density of states. It simplifies our task greatly.

Beyond the Born approximation (tube)

• First step: 2D effects. Nonlinear amplitude renormalization $\lambda \to \Lambda(\lambda)$ occurs already in nonrestricted geometry. Since scattering is isotropic (short-range) the unitarity theorem reads

Im
$$\Lambda = -|\Lambda|^2$$
, $\Lambda = \lambda e^{-i \arcsin \lambda}$

• Second step: boundary effects (topological). The Dyson equation for scattering operator T

$$T = V + Vg_0T$$
, $\Rightarrow T = \frac{V}{1 - Vg_0}$

• Here g_0 is the topologically nontrivial part of the single-point Green function. On a cylinder it is a contribution of **winding semiclassical trajectories**:

$$g_0(\varepsilon) = \sum_{n \neq 0} e^{\pi n \Phi / \Phi_0} \mathcal{G}_{\varepsilon}(2\pi nR) = \pi \sum_m (-\varepsilon_m)^{-1/2}$$

 $\mathcal{G}_arepsilon(r)$ - semiclassical Green function in 2D

Renormalized scattering amplitude

• Scattering amplitude

Scattering rate

$$\Lambda^{(\text{ren})} = \frac{\Lambda}{1 + \Lambda g(\varepsilon) / \pi v_0} \qquad \qquad \frac{1}{\tau(\varepsilon)} = \frac{2n}{\pi^2} \left| \frac{\Lambda}{1 + \Lambda g(\varepsilon) / \pi v_0} \right|^2 \frac{v(\varepsilon)}{v_0}$$

- For $|\varepsilon| \ll 1$ $\Lambda^{(ren)} \approx \lambda \{1 \Lambda/\pi \sqrt{\varepsilon}\}^{-1}$. Thus, non-Born single-impurity effects are essential if $\varepsilon < \varepsilon_{nB} = (\lambda/\pi)^2 \ll 1$
- On the other hand, the single-impurity non-Born effects can be destroyed by the multi-impurity Born scattering, if

$$\varepsilon_{\rm nB} < \varepsilon_{\rm min} = \left[(\lambda/\pi)^2 (n/\pi) \right]^{2/3}$$

• Finally, the criterion for ``non-Born regime" with strong single-impurity renormalization reads

$$n < n_c, \quad n_c = |\lambda|/\pi$$

Beyond the Born approximation (strip)

• The Green function $g_0(\varepsilon) \rightarrow g(\varepsilon, \xi_i)$ entering Dyson equation depends on the position of particular impurity:

$$g(\varepsilon,\xi_i) = -\mathcal{G}(2\xi_i) + \sum_{n=1}^{\infty} \left\{ 2\mathcal{G}(2n) - \mathcal{G}(2n+2\xi_i) - \mathcal{G}(2n-2\xi_i) \right\}$$
$$\approx -\frac{2\pi \sin^2(\pi N\xi_i)}{\sqrt{-\varepsilon}}$$

• Renormalized scattering amplitude depends on ξ_i either: $\Lambda_i^{(ren)} = \frac{\Lambda}{\Lambda_i}$

$$\Lambda_i^{(\text{ren})} = \frac{\Lambda}{1 + \Lambda g(\varepsilon, \xi_i) / \pi \nu_0}$$

• The scattering rate involves averaging over ξ_i

$$\frac{\tau_0}{\tau_{\rm nonres}(\varepsilon)} \approx \int_0^1 d\xi \frac{1 + 2\sin^2(\pi N\xi) \frac{\theta(\varepsilon)}{\pi\sqrt{\varepsilon}}}{\left|1 + 2\Lambda \sin^2(\pi N\xi)/\pi\sqrt{-\varepsilon}\right|^2}$$

• For $|\epsilon| \ll 1$ the average scattering is dominated by weak impurities with $\sin^2(\pi N\xi) \sim \sqrt{|\epsilon|} \ll 1$ 22



Resistivity $\rho(\varepsilon)$ in non-born regime: attracting impurities ($\lambda < 0$)



More about quasistationary states

• Positions of the poles in the scattering amplitude

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

- Finite width (imaginary part of energy) is due to escape to nonresonant bands
- Distribution function for binding energies (case of strip):

$$P(\varepsilon_{\rm qs}) = \frac{1}{\pi \sqrt{|\epsilon_{\rm qs}|(4 - |\epsilon_{\rm qs}|)}}$$

- Close to the left maximum (at $\epsilon_{qs} \approx -4$) scattering is dominated by quasistationary states at strong impurities with $\sin^2(\pi N\xi_i) \approx 1$
- Close to zero (at $|\epsilon| \ll 1$) scattering is dominated by quasistationary states at weak impurities with $\sin^2(\pi N\xi) \sim \sqrt{|\epsilon|} \ll 1$

Multi-impurity effects

• Multi-impurity effects are negligible for $\tau^{-1}(\varepsilon) < \varepsilon$ They become essential only at $\varepsilon < \varepsilon_{\min}^{(nB)}$, where $\varepsilon_{\min}^{(nB)}$ can be estimated from the condition

$$\tau^{-1} \left(\varepsilon = + \varepsilon_{\min}^{(nB)} \right) = \frac{2n}{\pi} \sqrt{\varepsilon_{\min}^{(nB)}} \sim \varepsilon_{\min}^{(nB)}$$

result
$$\varepsilon_{\min}^{(nB)} = (n/\pi)^2$$

• The behavior of asymptotics of $\tau^{-1}(\varepsilon)$

As a

$$\tau^{-1}(\varepsilon) = 2|\varepsilon|n\left(1 + \frac{1}{\pi\sqrt{\varepsilon}}\theta(\varepsilon)\right)$$

implies the existence of minimum of resistivity somewhere at $\varepsilon \sim \varepsilon_{\min}^{(nB)}$

• As in the Born case, asymptotics on different sides of singularity do not match:

$$\tau^{-1} \sim \begin{cases} n^2, \varepsilon > 0, \varepsilon \sim \varepsilon_{\min}^{(nB)} & \text{Again, it means that there should be a bifurcation point} \\ n^3, \varepsilon < 0, |\varepsilon| \sim \varepsilon_{\min}^{(nB)} & \text{near the minimum.} \end{cases}$$

Resistivity minimum: self-consistent approach

So far we have studied these effects only within the ``Self-consistent Non-Born Approximation'' (SCNBA). The SCNBA equation for the self-energy $\Sigma(\varepsilon)$ reads

$$\Sigma(\varepsilon) = \frac{n}{\pi^2} \left| \Lambda^{(\text{ren})}(\varepsilon - \Sigma(\varepsilon)) \right|^2 \frac{g(\varepsilon - \Sigma(\varepsilon))}{\pi v_0} \approx -in \left| \varepsilon - \Sigma \right| \left(1 + \frac{1}{\pi \sqrt{\varepsilon - \Sigma(\varepsilon)}} \right)$$



Conclusions

- High concentration of impurities $(n \gg n_e)$ Born single impurity scattering. Van Hove singularity structure: "plateau-maximum-plateau"
- Low concentration of impurities $(n \ll n_e)$ non-Born effects already in single impurity scattering.

Attracting impurities: "plateau-maximum-minimum-maximum- plateau" Important role of quasistationary states

Repulsing impurities: "plateau-minimum-maximum-plateau"

- Deep resistivity minimum near the Van Hove singularity (at $\varepsilon \sim n^2$). Without multi-impurity effects the minimal resistivity would be zero. With multi-impurity effects the minimal resistivity $\rho_{\min} \propto n$ is nonlinear in n
- Interesting mesoscopic physics is expected near the minimum.







