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Effects of impurity on the electronic properties of Luttinger semimetals

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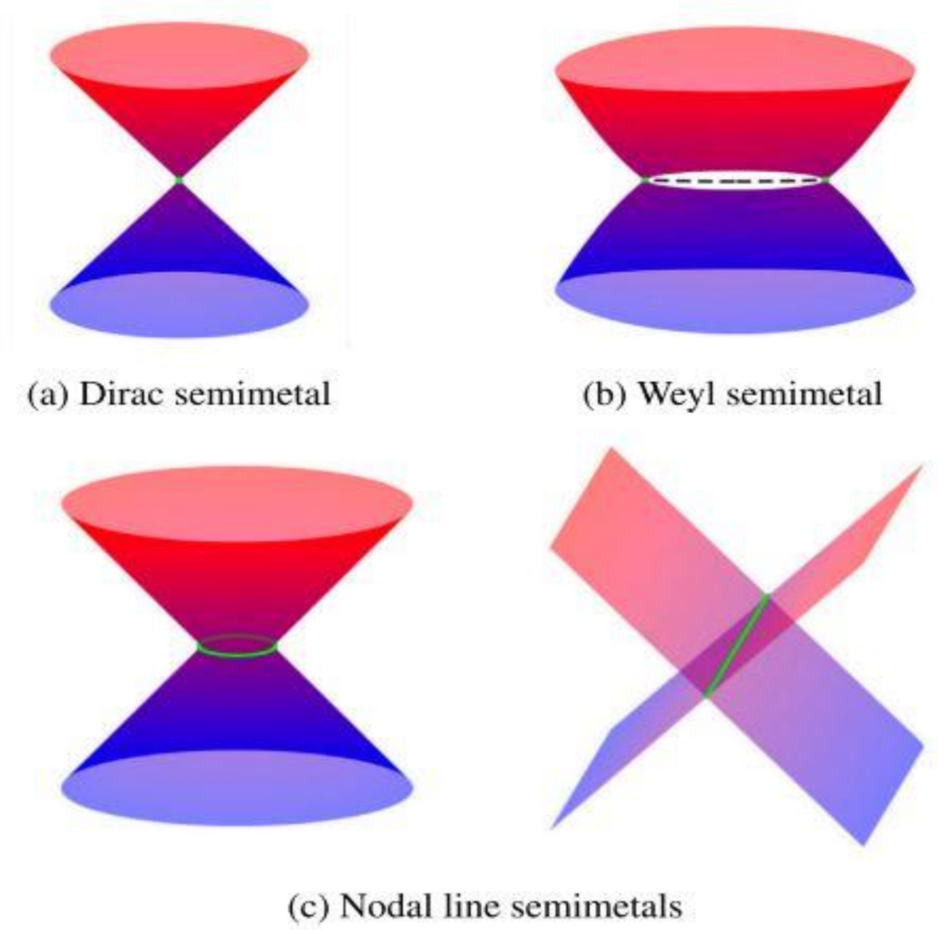
Outline

- Introduction
- Luttinger semimetals
- Green's function
- Results

Topological Semimetals (TS)

- Gapless topological material classification.
    - Dirac (DS)
    - Weyls (WS)
    - Nodal-line (NLS)
    - Luttinger semimetal (LS)



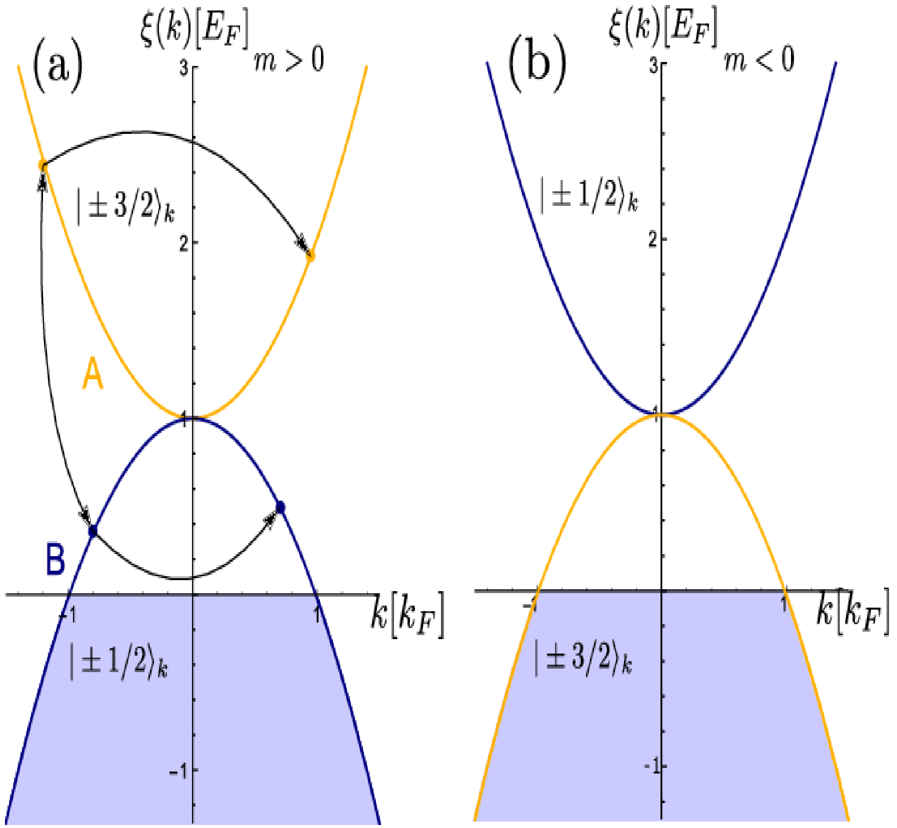
[1]. Yang, S. Y., Yang, H., Derunova, E., Parkin, S. S. P., Yan, B., & Ali, M. N. (2018). Symmetry demanded topological nodal-line materials. *Advances in Physics: X*, *3*(1). https://doi.org/10.1080/23746149.2017.1414631

Luttiger Semimetals (LS)

- LS hosts the excitation with effective spin- 3/2 .
- The $HgTe$, $\alpha - Sn$, $Pr_2rIr_2O_7$ and $YPtBi$.

$$H(\mathbf{k}) = \frac{\hbar^2}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)\mathbf{k}^2 - 2\gamma_2(\mathbf{k}.\mathbf{J})^2\right] \quad (1)$$

- In the case $|\gamma_1| < 2|\gamma_2|$



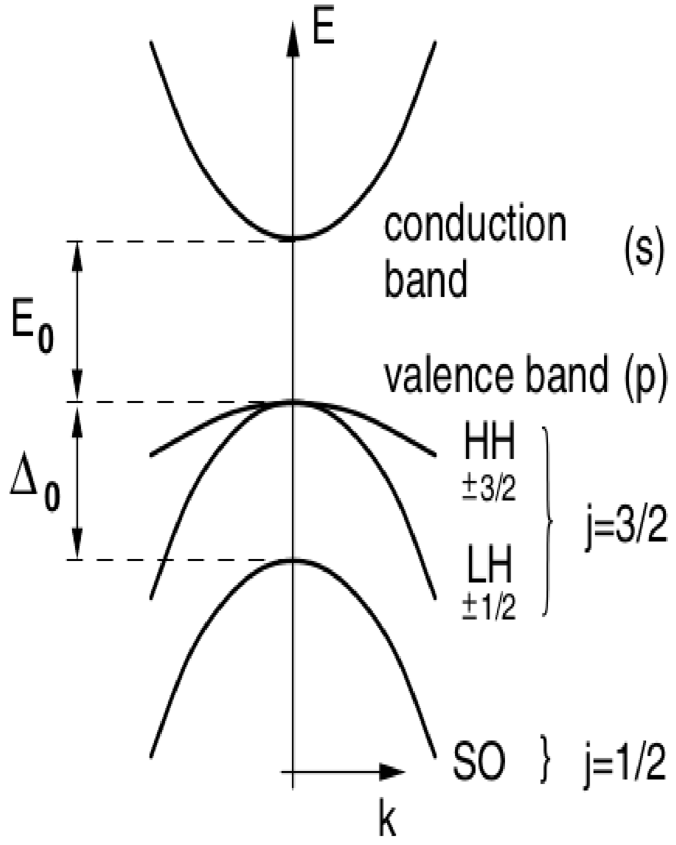
[2]. Mauri, Achille and Polini, Marco. Dielectric function and plasmons of doped three-dimensional luttinger semimetals. *Physical Review B*, 100(16):165115, 2019

Luttinger-Kohn $\boldsymbol{k.p}$ model (LK)

Considering the SOC at $k = 0$ every state is twofold degenerate $(X\uparrow, Y\uparrow, Z\uparrow)$ and $(X\downarrow, Y\downarrow, Z\downarrow)$ so we have a 6×6 Hamiltonian.

$$\mathcal{H}_{so} = \frac{\hbar}{4m^2c^2}(\sigma \times \nabla V)\cdot \mathbf{p} + \frac{\hbar}{4m^2c^2}(\sigma \times \nabla V)\cdot \boldsymbol{k} \qquad \textbf{(2)}$$

$$\mathcal{H}_{so} = \begin{pmatrix} P-Q & R & S & 0 & & \\ R^* & P-Q & 0 & S & \cdots & \langle SO|\mathbf{k.p}|HH,LH\rangle \\ S^* & 0 & P+Q & -R & & \\ 0 & S^* & -R^* & P+Q & & \\ & \vdots & & & \ddots & \vdots \\ & \langle HH,LH|\mathbf{k.p}|SO\rangle & & & \cdots & \begin{matrix} -\Delta+P & 0 \\ 0 & -\Delta+P \end{matrix} \end{pmatrix} \qquad \textbf{(3)}$$



[3]. Cukaric, Nemanja A. Modelling the electron and hole states in semiconductor nanostructures by the multiband k.p theory. *University of Belgrade*, 2015

Luttinger Hamiltonian (LH) in Spherical approximation

- **General form of LH**: products of j_x, j_y and j_x the component of j= $\frac{3}{2}$ produces 16 linearly independent matrix.

$$H(\mathbf{k}) = \frac{\hbar^2}{2m}\left[(\gamma_1 + \frac{5}{4}\gamma_2)\mathbf{k}^2 + 2\gamma_2(\mathbf{k}.\mathbf{J})^2 + 4(\gamma_2 - \gamma_3)\sum_{ij}\{k_i k_j\}\{J_i J_j\}\right]. \quad (4)$$

- **Spherical approximation** : In the case $\gamma_2 = \gamma_3$.

$$H(\mathbf{k}) = \frac{\hbar^2}{2m}\left[(\gamma_1 + \frac{5}{4}\gamma_2)\mathbf{k}^2 + 2\gamma_2(\mathbf{k}.\mathbf{J})^2\right]. \quad (5)$$

[4]. Luttinger, J Mi. Quantum theory of cyclotron resonance in semiconductors: General theory. *Physical Review*, 102(4):1030, 1956

Green's function and Born approximation

Green function used to solve DE in mathematic. While in QM it is a powerful tool for solving

$$[i\partial_t - H]\psi(\boldsymbol{r}, t) = 0 \qquad (6)$$

$$[i\partial_t - H]G(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\,\delta(t - t') \qquad (7)$$

The answer is

$$\psi(\mathbf{r}, t) = \int dr'\; G(\mathbf{r}t, \mathbf{r}'t')\,\psi(\mathbf{r}', t'). \qquad (8)$$

[5]. Bruus, Henrik and Flensberg, Karsten. *Many-body quantum theory in condensed matter physics: an introduction*. OUP Oxford, 2004.

Luttinger Hamiltonian Green's function

- Green's function for a given **Hamiltonian**:

$$[i\partial_t - H]G(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\,\delta(t - t') \tag{7}$$

So the **Furrier** transform is:

$$G(\mathbf{k}, \omega) = [\omega + i\eta - H(\mathbf{k})]^{-1} \tag{8}$$

- **Luttinger Hamiltonian** Green's function:

$$H_o(k) = \frac{\hbar^2}{2m}\left[\frac{5}{4}\mathbf{k}^2 - (\mathbf{k}.\mathbf{J})^2\right] - \xi_F \tag{9}$$

$$\Rightarrow \quad G_o\,(\mathbf{k}, \omega) = \frac{(\omega^+ + \xi_{\mathbf{F}})\gamma_o - \sum_i^5 h(k)\gamma_i}{(\omega^+ + \xi_{\mathbf{F}})^2 - {\xi_{\mathbf{k}}}^2} \tag{10}$$

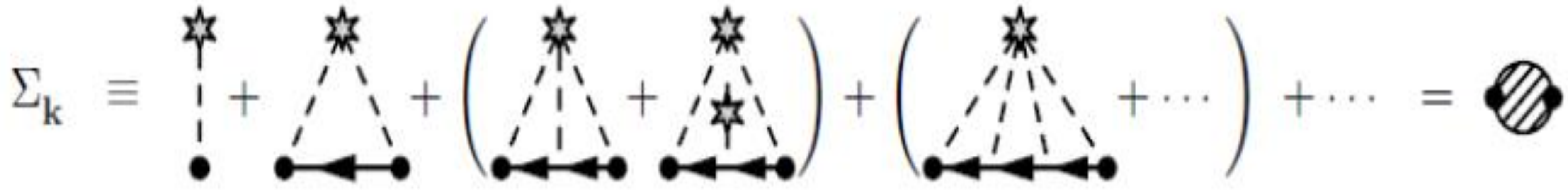
Self-energy

Interaction in the system :

$$G_0(\mathbf{k},\omega) = [\omega + i\eta - H_o(\mathbf{k})]^{-1} \quad (11)$$

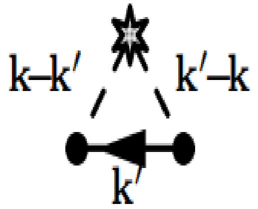
$$G_{in}(\mathbf{k},\omega) = [\omega + i\eta - H_o(\mathbf{k}) - \boldsymbol{V_{ex}}]^{-1} \quad (12)$$

$$G_{in}(\mathbf{k},\omega)^{-1} = G_0(\mathbf{k},\omega)^{-1} - \Sigma(i\omega) \quad (13)$$



Born approximation

- **First Born approximation**: this approximation contains the single scattering process:



$$\Sigma^{1BA}(i\omega) = \frac{\gamma_{imp}}{\text{V}} \sum_{\mathbf{k}'} u_{\mathbf{k}-\mathbf{k}'} G_0(\mathbf{k}', \omega) u_{\mathbf{k}'-\mathbf{k}} \qquad (14)$$

- **Self-consistent approximation**: we replace the interaction Green's function with the clean system.

$$\Sigma^{SCBA}(i\omega) = \frac{\gamma_{imp}}{\text{V}} \sum_{\mathbf{k}'} u_{\mathbf{k}-\mathbf{k}'} \, G_{in}(\mathbf{k}, \omega) \, u_{\mathbf{k}'-\mathbf{k}} \qquad (15)$$

$$G_{in}(\mathbf{k}, \omega)^{-1} = G_0(\mathbf{k}, \omega)^{-1} - \Sigma^{SCBA}(i\omega) \qquad (16)$$

First Borrn approximation

- Impurity:

$$U = u_0 \sum_{i}^{N_{imp}} \delta(\mathbf{r} - R_i) \tag{17}$$

$$\Sigma^{1BA}(i\omega) \;\; = \frac{\gamma_{imp}}{\mathrm{V}} \sum_{\mathbf{k}'} u_{\mathbf{k}-\mathbf{k}'} G_0(\mathbf{k}', \omega) u_{\mathbf{k}'-\mathbf{k}} \tag{18}$$

$$\Sigma^{1BA}(i\omega) \;\; = \frac{\gamma_{imp} {u_0}^2}{2\pi^2} \times \frac{1}{2} \int_0^{\alpha} k^2 dk \left[\frac{1}{\hbar\omega + i\eta + \xi_{\mathbf{F}} - \xi_{\mathbf{k}}} + \frac{1}{\hbar\omega + i\eta + \xi_{\mathbf{F}} + \xi_{\mathbf{k}}} \right] \tag{19}$$

$$\frac{1}{x \pm i\boldsymbol{y}} = \mathrm{P}\left(\frac{1}{x}\right) \mp i\pi\delta(x) \tag{20}$$

○ **Real part** :

$$\mathbf{Re}\Sigma^{1BA}(\hbar\omega) \;\; = \frac{\gamma_{imp}{u_0}^2}{2\pi^2} \times \frac{1}{2}\int_0^{\alpha} k^2 dk \, [\frac{1}{\hbar\omega + \xi_{\mathbf{F}} - \xi_{\mathbf{k}}} + \frac{1}{\hbar\omega + \xi_{\mathbf{F}} + \xi_{\mathbf{k}}}]$$

$$\mathbf{Re}\Sigma^{1BA}(\hbar\omega) \;\; = -U\sqrt{|\hbar\omega + \xi_{\mathbf{F}}|} \qquad (21)$$

○ **Imaginary part**:

$$\mathbf{Im}\Sigma^{1BA}(\hbar\omega) \;\; = -\frac{\gamma_{imp}{u_0}^2}{4\pi}\int_0^{\alpha} k^2 dk \, [\delta(\hbar\omega + \xi_{\mathbf{F}} - \xi_{\mathbf{k}}) + \delta(\hbar\omega + \xi_{\mathbf{F}} + \xi_{\mathbf{k}})\,]$$

$$\mathbf{Im}\Sigma^{1BA}(\hbar\omega) = -U\sqrt{|\hbar\omega + \xi_{\mathbf{F}}|} \qquad (22)$$

Where $U = \frac{\gamma_{imp}{u_0}^2}{8\pi} \times (\left|\frac{2m}{\hbar^2}\right|)^{\,3/2}$

Self-consistent approximation

$$\begin{cases} \Sigma^{SCBA}(i\omega) = \frac{\gamma_{imp}}{\mathrm{V}} \sum_{\mathbf{k}'} u_{\mathbf{k}-\mathbf{k}'} G_{in}(\mathbf{k}', \omega) u_{\mathbf{k}'-\mathbf{k}} \\ G_{in}(\mathbf{k}, \omega)^{-1} = G_0(\mathbf{k}, \omega)^{-1} - \mathbf{\Sigma}^{SCBA}(i\omega) \end{cases}$$

- So we have :

$$\mathbf{\Sigma}^{SCBA}(i\omega) \quad = \frac{\gamma_{imp} {u_0}^2}{2\pi^2} \int_0^{\alpha} k^2 dk \left[\frac{\hbar\omega + i\eta + \xi_{\mathbf{F}} - \mathbf{\Sigma}^{SCBA}(i\omega)}{\left(\hbar\omega + i\eta + \xi_{\mathbf{F}} - \mathbf{\Sigma}^{SCBA}(i\omega)\right)^2 - {\xi_{\mathbf{k}}}^2} \right] \qquad (23)$$

$$\mathbf{\Sigma}^{SCBA}(i\omega) \quad = -U(i+1)\sqrt{|\hbar\omega + \xi_{\mathbf{F}}| - \mathbf{\Sigma}^{SCBA}(i\omega)} \qquad (24)$$

After solving this equation we found the real an imaginargy part of the self-energy in the self-consistent approximation.

$$\mathbf{\Sigma}^{SCBA}(i\omega) \quad = -U(i+1)\sqrt{|\hbar\omega + \xi_{\mathbf{F}}| - \mathbf{\Sigma}^{SCBA}(i\omega)}$$

○ **Real part** :

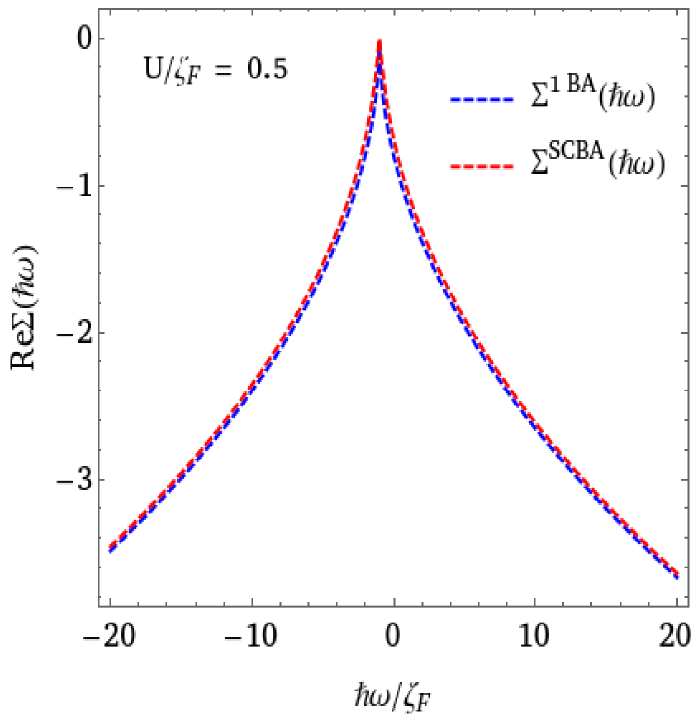
$$\mathbf{Re\Sigma}^{SCBA}(i\omega) = -\frac{U|\hbar\omega + \xi_{\mathbf{F}}|\sqrt{2}}{\sqrt{U^2 + \sqrt{U^4 + 4(|\hbar\omega + \xi_{\mathbf{F}}|)^2}}} \tag{25}$$

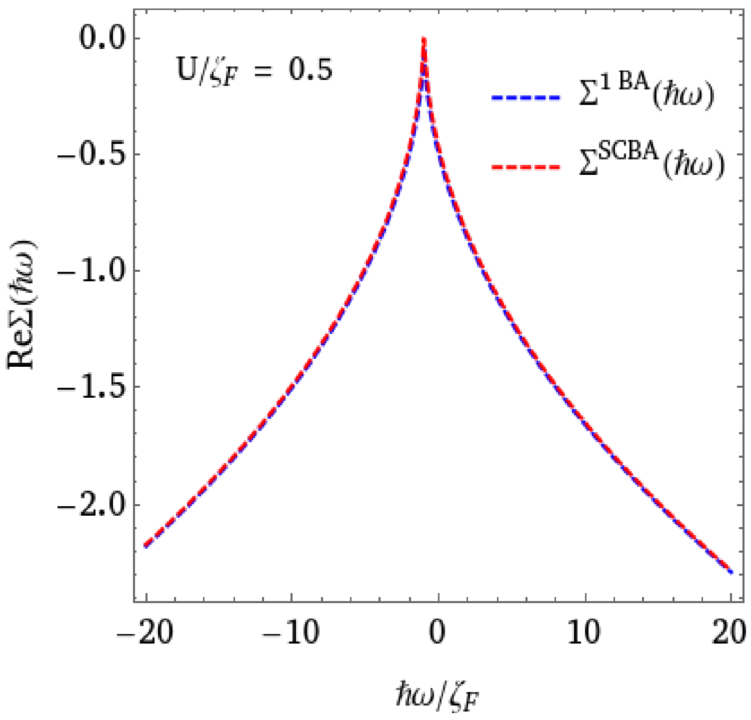
○ **Imaginary part**:

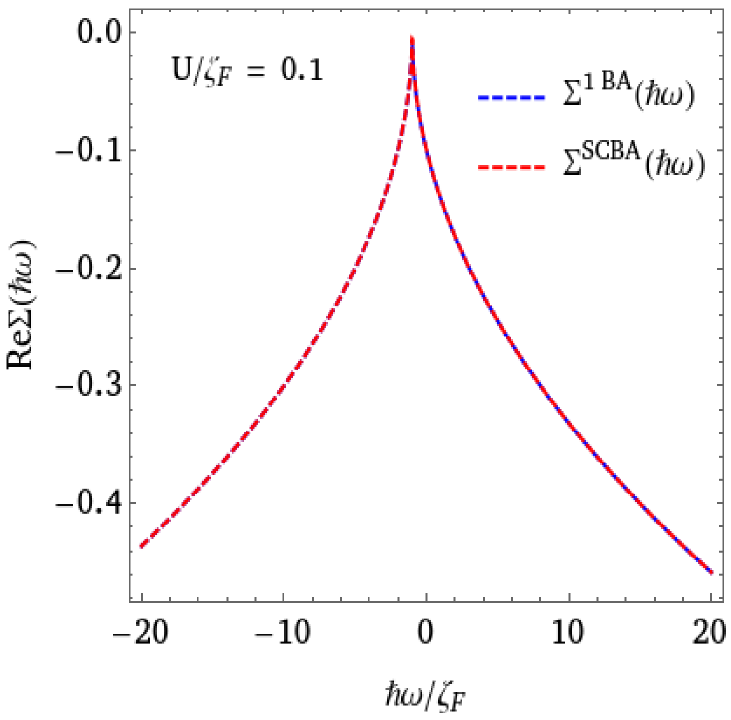
$$\mathbf{Im\Sigma}^{SCBA}(i\omega) = -\frac{\sqrt{3U^4 + U^2\sqrt{U^4 + 4(|\hbar\omega + \xi_{\mathbf{F}}|)^2} + 2U^2\sqrt{2U^4 + 2U^2\sqrt{U^4 + 4(|\hbar\omega + \xi_{\mathbf{F}}|)^2}}}}{\sqrt{2}} \tag{26}$$

Self-energy Real part in 1BA and SCBA

Real part of Self-energy plot as function of frequency in unit of Fermi energy.

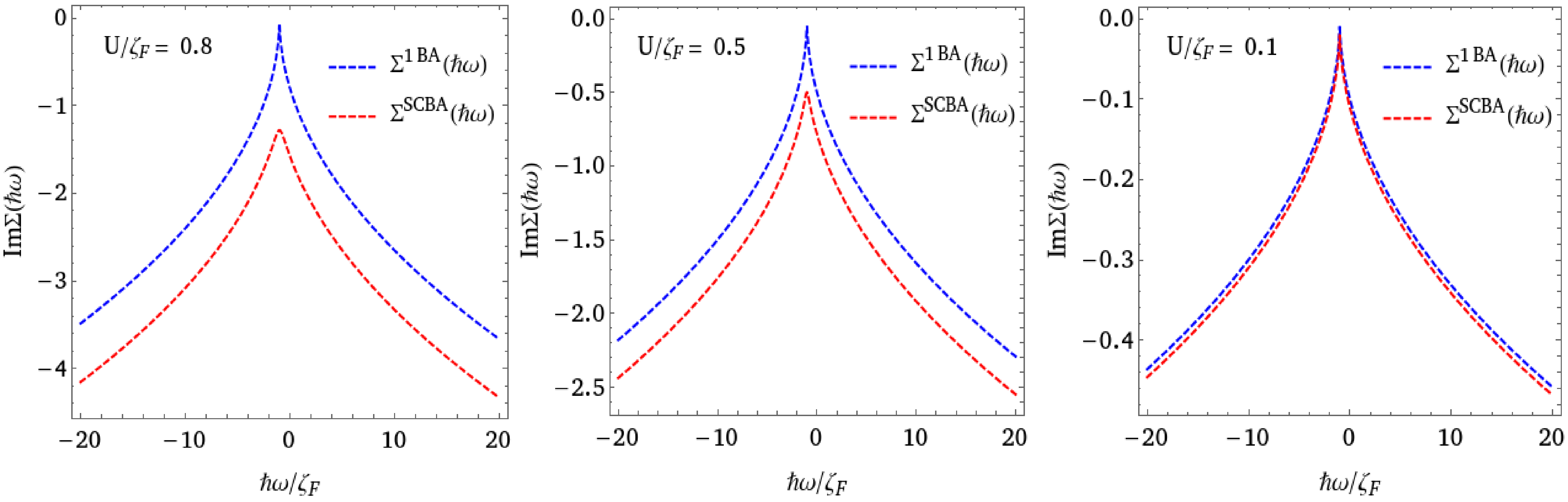






Self-energy Imaginary part in 1BA and SCBA

Imaginary part of Self-energy plot as function of frequency in unit of Fermi energy.



Spectral function

According to definition:

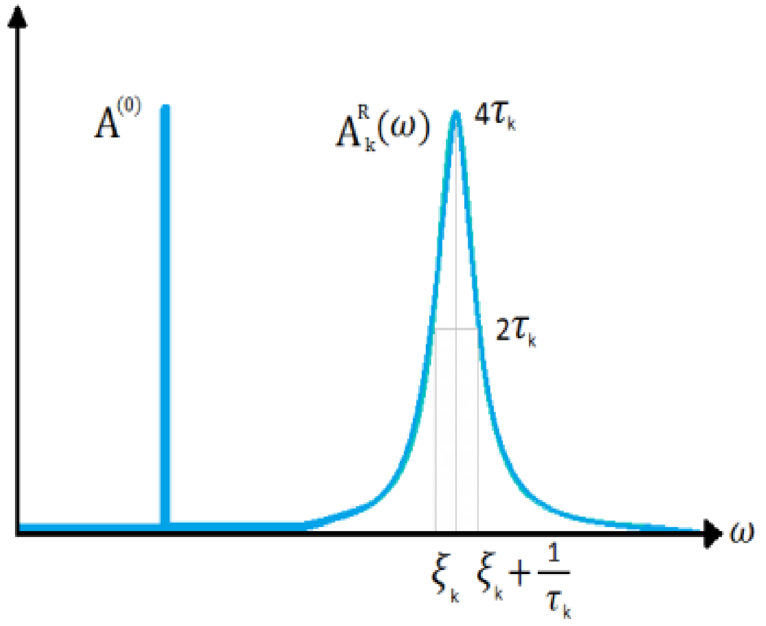
$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathbf{Im}TrG(\mathbf{k},\omega)$$

For Free particles the Green's function is as fallow :

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \xi_{\mathbf{k}}} \quad \Rightarrow \quad A(\mathbf{k},\hbar\omega) = \delta(\omega + \xi_{\mathbf{k}})$$

$$G^R(\mathbf{k},\omega) \approx -i\theta(t)e^{-i\xi_{\mathbf{k}}t}e^{-t/\tau}$$

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathbf{Im}\int dt\ e^{i\omega t}G^R(\mathbf{k},\omega) \approx \frac{1/\tau}{(\omega - \xi_{\mathbf{k}})^2 - (t/\tau)^2}$$



(LS)'s Spectral function in the presence of Impurity

According to definition the clean system Spectral function is

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathbf{Im}TrG(\mathbf{k},\omega)$$

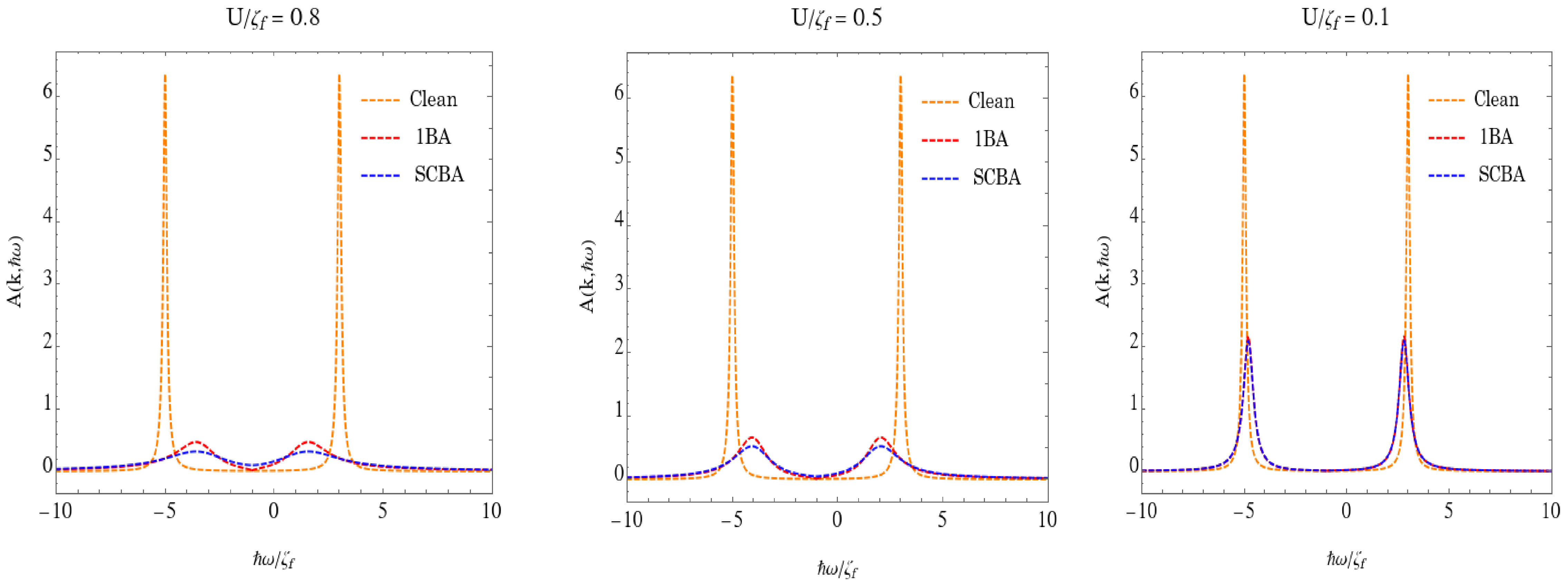
$$A(\mathbf{k},\hbar\omega) = 2[\delta(\hbar\omega + \xi_{\mathbf{F}} - \xi_{\mathbf{k}}) + \delta(\hbar\omega + \xi_{\mathbf{F}} + \xi_{\mathbf{k}})] \quad (27)$$

In the interaction case(note that here $\acute{\xi}_{\mathbf{k}} = \xi_{\mathbf{k}} - \mathbf{Re}\Sigma(\hbar\omega)$:

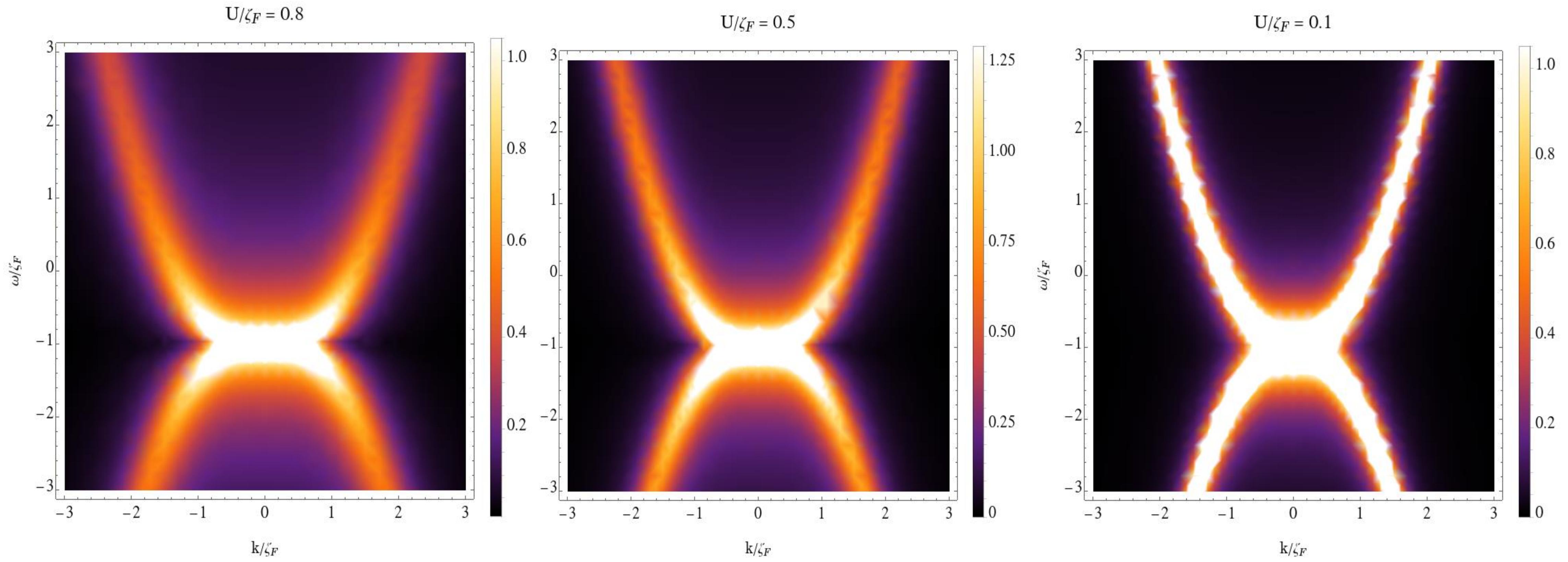
$$A(\mathbf{k},\omega) = -\frac{2}{\pi}\left[\frac{\mathbf{Im}\Sigma(\hbar\omega)}{\left(\hbar\omega+\xi_{\mathbf{F}}-\acute{\xi}_{\mathbf{k}}\right)^2+\mathbf{Im}\Sigma(\hbar\omega)^2} + \frac{\mathbf{Im}\Sigma(\hbar\omega)}{\left(\hbar\omega+\xi_{\mathbf{F}}+\acute{\xi}_{\mathbf{k}}\right)^2+\mathbf{Im}\Sigma(\hbar\omega)^2}\right] \quad (28)$$

(LS)'s Spectral function in the presence of Impurity

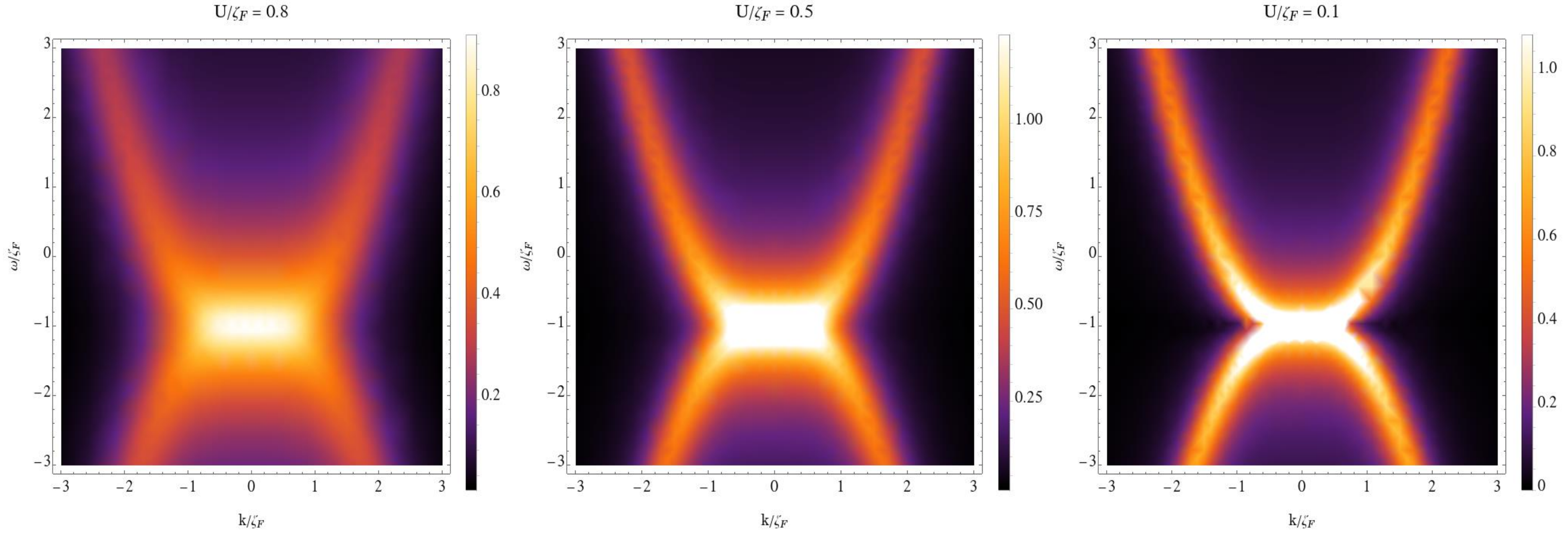
Spectral function for a constant wave vector:



LS's Spectral function intensity in the 1BA



(LS)'s Spectral function intensity in the SCBA



Density of States (DOS)

- **Definition:**

According to definition we can calculate the DOS from the Green's function for the following relation:

$$\mathrm{D}(\xi) = -\frac{g_s}{V}\sum_{i}^{n} \delta(\xi + \xi_i(\mathbf{k}))$$

Using the Green's function :

$$\mathrm{D}(\xi) = -\frac{g_s}{\pi}\frac{1}{V}\sum_{\mathbf{k}} \mathbf{Im} TrG(\mathbf{k}, \omega)$$

LS's DOS in the presence of impurity

- So the DOS of Luttinger Semimetals (LS) in the in absence of the impurity is:

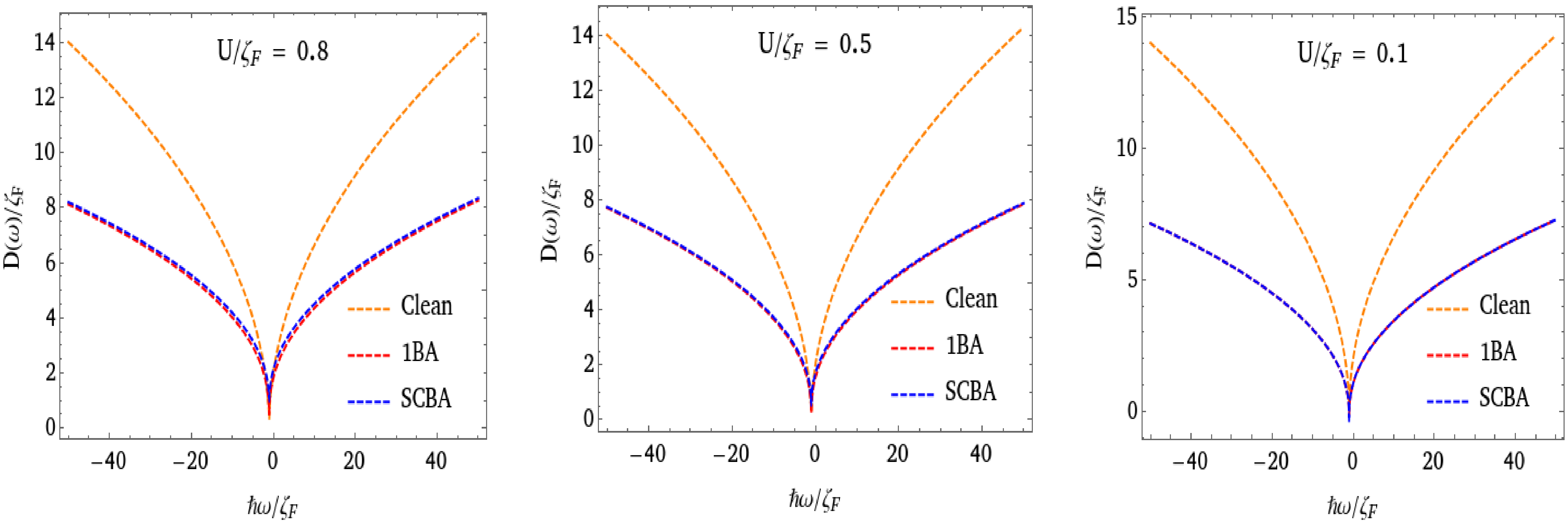
$$\mathrm{D}(\xi) = -\frac{g_s}{V}\sum_{\mathbf{k}} \boldsymbol{A}(\mathbf{k}, \omega) \quad = D_o\sqrt{|\hbar\omega + \xi_{\mathbf{F}}|}$$

- In the presence of impurity:

$$\mathrm{D}(\xi) = -\frac{D_o}{2}\frac{|\hbar\omega + \xi_{\mathbf{F}}| - \mathbf{Re}\Sigma(\hbar\omega) + \mathbf{Im}\Sigma(\hbar\omega)}{\left[\left(|\hbar\omega + \xi_{\mathbf{F}}| - \mathbf{Re}\Sigma(\hbar\omega)\right)^2 + \mathbf{Im}\Sigma(\hbar\omega)^2\right]^{\frac{1}{4}}}$$

Where $D_o = \frac{g_s}{\pi^2} \times \left(\left|\frac{2m}{\hbar^2}\right|\right)^{3/2}$

LS's DOS in presence of Impurity



Thank you!