Friedel Oscillations and Weak Interaction in 1D and Higher Dimensions

1. Friedel oscillations created by a single impurity in 1D

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1. Friedel oscillations in 1D.

Consider a point-like impurity in a 1D spinless free Fermi gas. The set of eigenfunctions in its presence can be written as:

$$\varphi_k(x) = (1/\sqrt{2\pi}) \begin{cases} e^{ikx} + r_0 e^{-ikx}, & x<0 \\ t_0 e^{ikx}, & x>0 \end{cases} \quad \text{(states incoming from left)} \qquad (56)$$

and

$$\varphi_{-k}(x) = \frac{1}{\sqrt{2\pi}} \begin{cases} t_0 e^{-ikx}, & x<0 \\ e^{-ikx} + r_0 e^{ikx}, & x>0 \end{cases} \qquad (57)$$

$(k>0)$. We neglect the k-dependence of the transmission and reflection amplitude (t_0, r_0) taking their values at $k=k_F$.

We may evaluate the average density, $n(x) = \sum_{|k|<k_F} |\varphi_k(x)|^2$, as

$$n(x) = \begin{cases} n_0 + \frac{1}{\pi}\int_0^{k_F} dk \, \mathrm{Re}\{r_0 e^{-2ikx}\}, & x<0 \\ n_0 + \frac{1}{\pi}\int_0^{k_F} dk \, \mathrm{Re}\{r_0^* e^{-2ikx}\}, & x>0 \end{cases} \qquad (58)$$

At large distance from the impurity, $|x| \gg \lambda_F$, the density perturbation

$$\delta n(x) = n(x) - n_0 \simeq \frac{|r_0|}{2\pi |x|} \sin(2k_F|x| + \arg r_0) \qquad (59)$$

This is the 1D version of the Friedel oscillations of density.

2. Scattering off the Friedel oscillation.

In the presence of interaction, the oscillation of density produces an oscillatory (decaying) potential, $V_H(x) \sim V(2k_F) \cdot \delta n(x) \propto \sin(2k_F|x| - \arg r_0)/|x|$. Note that such a potential may lead to log-divergent ~~correction~~ Born amplitude of backscattering, as

$$\int_{\lambda_F}^{\infty} \frac{dx}{x} e^{2i(k-k_F)x} \sim \ln \frac{1}{\lambda_F \cdot |k-k_F|} \qquad (60)$$

Having this hint, we do the calculation more carefully. To the first order in the interaction $V(x-y)$ (and any t_0, r_0),

$$\psi_k(x) = \varphi_k(x) + \int dy\, G_k(x,y) \int dz \left\{ V_H(z)\,\delta(y-z) + V_{ex}(y,z) \right\} \varphi_k(z) \qquad (61)$$

Here

$$V_H(x) = \int dy\, V(x-y)\, n(y), \qquad (62)$$

see Eq. (58) for $n(y)$, and

$$V_{ex}(x,y) = -V(x-y) \sum_{|k|<k_F} \varphi_k^*(y)\, \varphi_k(x). \qquad (63)$$

Eventually we will be interested in modifications to the transmission, so let us concentrate on the $x \to \infty$ asymptote for $\psi_k(x)$, $k>0$. The corresponding form of the Green function is

$$G_k(x,y) = \frac{1}{i v_k} \begin{cases} t_0 e^{ik(x-y)}, & y<0 \\ e^{ik(x-y)} + r_0 e^{ik(x+y)}, & y>0 \end{cases} \qquad (64)$$

Casting the asymptote in the form $\Psi_k(x) = (1/\sqrt{2\pi})\, t_k e^{ikx}$, $x \to +\infty$, we find from Eqs. (61)–(64):

$$t_k = t_0 - \gamma t_0 |r_0|^2 \ln\left|\frac{1}{(k-k_F)\cdot d}\right|, \quad \gamma = \frac{\overset{\text{exchange}}{V(0)} - \overset{\text{Hartree}}{V(2k_F)}}{2\pi v_F} \qquad (65)$$

(here d is the impurity "size" or λ_F). In accord with expectations, Eq. (60) the correction to the amplitude is <u>divergent</u> at $k \to k_F$.

Here is a pictorial view of "making" of the correction to t_0:

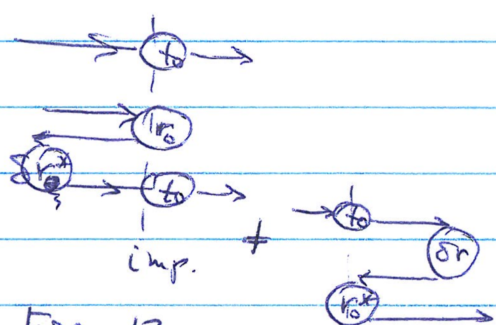


Fig. 12

It is clear from Fig. 12 that $t_k - t_0$ <u>must</u> be $\propto t_0 \cdot |r_0|^2$.
The log-divergence comes from long distances, $|x| \gg \lambda_F$ in Eq. (60), so only the cut-off in Eq. (65) is model-dependent. A monotonic repulsive interaction ($V(0) > V(2k_F) > 0$) leads to a suppression of the transmission.

3. RG for the elastic backscattering.

Now we want ~~to~~ to "cure" the divergence of the backscattering correction, Eq. (65). Note that at $\gamma \ll 1$ the spatial scale producing the divergence is exponentially large. We will use it to develop a "real-space" RG allowing us to sum-up the leading-log series, $\sum_n c_n \gamma^n \ln^n \ldots$.

Let us split the interval $[d, 1/|k-k_F|]$ contributing to the log-divergent integrals of the type Eq.(60) on smaller pieces such that $l_n - l_{n-1} \gg d$, but $\gamma \int_{l_{n-1}}^{l_n} \frac{dx}{x} \ll 1$.

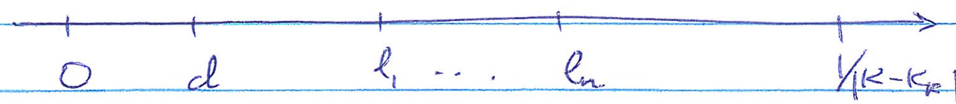


Fig. 13

We may replace the initial problem with scattering amplitudes t_0, r_0 by a new one, where the scatterer is replaced by the "bare" one + Friedel oscillation over a scale $|x| < l_1$. The scattering amplitude of such "composite" scatterer is

$$t_1 = t_0 - \gamma t_0 (1 - |t_0|^2) dl, \qquad (65)$$

where $dl = \ln(l_1/d)$. We may keep repeating this procedure, yielding

$$t_{n+1} = t_n - \gamma t_n (1 - |t_n|^2) dl, \quad dl = \ln \frac{l_{n+1}}{l_n} \qquad (67)$$

The iterations stop at such n that $l_n = 1/|k-k_F|$. Taking all $l_n - l_{n-1}$ equal each other and implementing the continuous limit, we get

$$\frac{dt}{dl} = -\gamma t (1 - |t|^2), \quad l = \ln \frac{L}{d}; \qquad (68)$$

The boundary condition for this RG equation is $t(l=0) = t_0$, and the integration stretches to $l = \ln(1/|k-k_F| d)$

Reviews: MPA Fisher, LG, Transport in a 1D Luttinger liquid, in: L.L. Sohn et al (eds.), Mesoscopic Electron Transport, 1997 Kluwer, pp 331–373

Upon integration of Eq. (68), we find the transmission coefficient as a function of energy ε measured from the Fermi level:

$$\boxed{T(\varepsilon) = \frac{T_0 \cdot |\varepsilon/D_0|^{2\gamma}}{R_0 + T_0|\varepsilon/D_0|^{2\gamma}}}, \tag{69}$$

where $T_0 = 1 - R_0 = |t_0|^2$ and $D_0 = v_F/d$ are bare parameters of the problem. Now we may use Landauer formula,

$$G = \frac{e^2}{2\pi\hbar}\int d\varepsilon\left(\frac{\partial f}{\partial \varepsilon}\right)T(\varepsilon), \quad f(\varepsilon) = \frac{1}{e^{\varepsilon/T}+1} \tag{70}$$

to evaluate $G(T)$. At $\gamma \ll 1$, the factor $\partial f/\partial\varepsilon$ is the sharpest function of energy of the two factors in the integrand;

$\Downarrow$

$$G(k_BT) = \frac{e^2}{2\pi\hbar}\cdot\frac{T_0\,(k_BT/D_0)^{2\gamma}}{R_0 + T_0\,(k_BT/D_0)^{2\gamma}} \tag{71}$$

We see that at $T \to 0$ (or at $\varepsilon \to 0$ in Eq. (69)) the ~~trans~~ conductance (transmission) vanishes as a power law, $T(\varepsilon) \propto \varepsilon^{2\gamma}$ in agreement with the bosonization picture (Kane, Fisher, PRL 68 1220 (92)); moreover the exponent γ does coincide with $\frac{1}{K} - 1$ if one expands K in powers of interaction (retaining V^0, V^1).

The most telling case of Eq. (69) is $R_0 \ll 1$, allowing for a strong change of $T(\varepsilon)$ at $\varepsilon \ll D_0$. The

crossover function can be cast in a scaling form:

$$T(\varepsilon) = \frac{(\varepsilon/\varepsilon^*)^{2\gamma}}{1+(\varepsilon/\varepsilon^*)^{2\gamma}}, \quad R(\varepsilon) = \frac{(\varepsilon^*/\varepsilon)^{2\gamma}}{1+(\varepsilon^*/\varepsilon)^{2\gamma}}; \; \varepsilon^* = D_0\left(\frac{R_0}{T_0}\right)^{1/2\gamma}. \quad (72)$$

Scaling limit is $D_0 \to \infty$, $(R_0/T_0)^{1/2\gamma} \to 0$ at γ and ε^* finite, fixed; $\varepsilon^* = D_0(R_0/T_0)^{1/2\gamma}$. The "high-energy" end of $R(\varepsilon)$ from Eq. (72) can also be matched to the Kane and Fisher [KF] work:

$$R(\varepsilon) \sim \left(\frac{\varepsilon}{\varepsilon^*}\right)^{-2\gamma} \Longleftrightarrow R(\varepsilon) \propto \varepsilon^{2(K-1)} \; [KF] \quad (73)$$

at $1-K \to \gamma$ (weak interaction limit)

Equations (69)-(72) are valid as long as $T, \varepsilon \gtrsim \hbar v_F/L$ and are cut off at that energy due to the finite system size.

Consider now a finite-length (L) wire with an impurity density n_{imp}. Neglecting interference, the mean free path of electron with energy ε is found from:

$$\frac{1}{\ell(\varepsilon)} = n_{imp} \cdot R(\varepsilon) \quad (74)$$

and the resistance is $\mathbb{R}(T, L) \sim L/\ell(\varepsilon\sim T) = n_{imp} L \cdot R(\varepsilon \sim T)$, as long as $T \gtrsim \hbar v_F/L$. At lower temperatures,

$$\mathbb{R}(T, L) \sim n_{imp} \cdot L \cdot \left(\frac{\hbar v_F}{L}\right)^{2(K-1)} \propto \left(\frac{1}{L}\right)^{2K-3} \quad (75)$$

(we used the generalization $\gamma \to 1-K$, see Eq.(73), here).

At $K=3/2$ (corresponding to a pretty strong attraction between fermions) $\mathbb{R}(L_i)$ becomes L-independent signalling a transition from localized to a delocalized phase (see Lectures by Giamarchi).

Rudin et. al. PRB 55, 9322 (1997)

4. Friedel Oscillations in Higher Dimensions: ZBA in DOS.

Singular backscattering off the Friedel oscillation persists in higher dimensions, leading to non-analytical corrections to the tunneling density of states (DOS) and conductivity. ⇒ We illustrate the role of Friedel oscillations by examining the interaction-induced correction to DOS, $\delta\nu(\varepsilon)$, at $\varepsilon > \hbar/\tau$ in 2D (here τ is elastic mean free path caused by impurities of density n_i and potential

$$U_{imp}(\vec{r}-\vec{r}_i) = g\,\delta(\vec{r}-\vec{r}_i) \tag{76}$$

A single impurity at origin ($\vec{r}_i=0$) creates a Friedel oscillation of density

$$\delta n(r) = n(r) - n_0 = \sum_{\varepsilon_\ell<0} |\psi_\ell(\vec{r})|^2 - n_0 = -\frac{\nu_0 g}{2\pi}\,\frac{\sin(2k_F r)}{r^2} \tag{77}$$

(we assume weak potential Eq. (76); $k_F r \gg 1$).

In the presence of interaction, similar to Eqs. (62), (63), ~~we have~~ additional source of scattering: ~~the~~ $\delta n(r)$ creates an

$$H_{HF}(\vec{r}_1,\vec{r}_2) = V_H(\vec{r}_1)\,\delta(\vec{r}_1-\vec{r}_2) - V_{ex}(\vec{r}_1,\vec{r}_2)$$

$$V_H(\vec{r}) = \int d\vec{r}_1\, \delta n(\vec{r}_1)\, V(\vec{r}-\vec{r}_1) \qquad (78)$$

$$V_{ex} = V(\vec{r}_1-\vec{r}_2)\cdot\frac{1}{2}\sum_{\varepsilon_\ell<0}\psi_\ell^*(\vec{r}_2)\,\psi_\ell(\vec{r}_1)$$

(spin is included; $V(\vec{r})$ is a short-range interaction).

The *local* DOS is $\nu(\varepsilon,\vec{r}) = -(2/\pi)\,\mathrm{Im}\,G^R(\varepsilon,\vec{r},\vec{r})$. Motivated by Eq. (65) and Fig. 12, we examine now the cross-term of the correction $\delta G^R(\varepsilon,\vec{r},\vec{r})$ coming from scattering off impurity potential, Eq. (76), *and* the Friedel oscillation, Eq. (78):

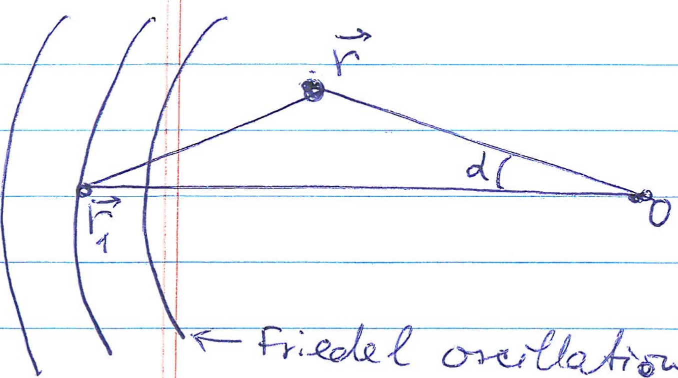
$$\delta G^R(\varepsilon,\vec{r},\vec{r}) = 2g\Big\{G^R(\varepsilon,r,0)\int G^R(\varepsilon,0,\vec{r}_1)\,V_H(\vec{r}_1)\,G^R(\varepsilon,\vec{r}_1,\vec{r})\,d\vec{r}_1$$

$$-\,G^R(\varepsilon,\vec{r},0)\int G^R(\varepsilon,0,\vec{r}_1)\,V_{ex}(\vec{r}_1,\vec{r}_2)\,G^R(\varepsilon,r_2,r)\,dr_1\,dr_2\Big\}. \qquad (79)$$

The free-fermion Green function in 2D at $k_F|\vec{r}_1-\vec{r}_2|\gg 1$ and $|\varepsilon|\ll E_F$ is

$$G(\varepsilon,\vec{r}_1,\vec{r}_2) = \frac{m\,e^{i\pi/4}}{\hbar^2\sqrt{2\pi k_F|\vec{r}_1-\vec{r}_2|}}\,e^{i\left(k_F+\frac{\varepsilon}{\hbar v_F}\right)|\vec{r}_1-\vec{r}_2|} \qquad (80)$$

The leading contribution to the integrals in Eq. (79) comes from small angles, $\alpha \lesssim \sqrt{\lambda_F/r}$, see Fig. 13. We explain that concentrating on the Hartree term in Eq. (79).



← Friedel oscillations of density (and $V_H(\vec{r})$)

Fig. 13

Indeed, the product entering the first term there,

$$G^R(r,0)\cdot G^R(0,r_1)\cdot G^R(r_1,r) \propto \exp[i\varphi(\vec{r},\vec{r}_1)], \quad (81)$$

where the phase

$$\varphi(\vec{r},\vec{r}_1) = (r + r_1 + |\vec{r}-\vec{r}_1|)(k_F + \varepsilon/\hbar v_F), \quad (82)$$

cf. Eq. (80). Another strongly oscillatory factor in that term is $V_H(\vec{r}_1) \propto \sin(2k_F r_1)$. The total phase of the integrand, $\varphi(\vec{r},\vec{r}_1) - 2k_F r_1$, is a slow function of $\vec{r}_1$ for the angles $\alpha < \sqrt{\lambda_F/r}$:

$$\varphi(\vec{r}\vec{r}_1) - 2k_F r_1 \sim 2(\varepsilon/\hbar v_F)\cdot r_1 \quad (83)$$

Integration in Eq. (79) yields:

$$\delta\nu(\varepsilon,\vec{r}) \simeq -\frac{[V(0)-2V(2k_F)]\nu_0^2 g^2}{r^2}, \quad \lambda_F \lesssim r \lesssim \hbar v_F/\varepsilon; \quad (84)$$

(at $r \lesssim \lambda_F$ ~~δ~~ correction remains finite; at $r \gtrsim \hbar v_F/\varepsilon$, correction $\propto 1/r^3$).

Note that $\delta\nu(\varepsilon,\vec{r})$ <u>does not</u> oscillate with $\vec{r}$.

Averaging over $\vec{r}$ and summing over impurities, we get

$$\frac{\langle\delta\nu(\varepsilon,\vec{r})\rangle}{\nu_0} = -\frac{[V(0)-V(2k_F)]\nu_0\hbar}{4\pi E_F\tau}\ln\left(\frac{E_F}{\varepsilon}\right); \quad \tau^{-1} = \frac{2\pi}{\hbar}\nu_0 n_i g^2. \quad (85)$$

(a singular correction to ν_0).

5. Interaction correction to DOS in the diffusive limit.

Above we considered first scattering off a single impurity and its Friedel oscillation, and then summed over impurities. At high impurity density (or, rather, at $\varepsilon\tau \ll \hbar$) we better express $V_H(\vec{r})$ and $V_{ex}(\vec{r}_1, \vec{r}_2)$ of Eq. (78) in terms of the Green function $\mathcal{G}^R_\varepsilon(\vec{r}_1, \vec{r}_2)$ accounting for the impurities. Then, instead of Eq. (79) we evaluate the <u>first-order</u> correction in V_{ex}, V_H (while impurities are already accounted in $\mathcal{G}^R_\varepsilon$):

$$\delta \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}) = \int d\vec{r}_1\, \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}_1) V_H(\vec{r}_1)\, \mathcal{G}^R_\varepsilon(\vec{r}_1, \vec{r}) - \int \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}_1) V_{ex}(\vec{r}_1, \vec{r}_2)\, \mathcal{G}^R_\varepsilon(\vec{r}_2, \vec{r})\, d\vec{r}_1 d\vec{r}_2 . \tag{86}$$

We are interested in $\delta\nu(\varepsilon) = (1/V_d)\int d^d\vec{r}\, \delta\nu(\varepsilon, \vec{r})$.

Let us concentrate on the Hartree contribution (first term in Eq. (86)) and a finite-range potential, for illustration. With the help of an easy-to-check identity, $\int dr\, \mathcal{G}^R_\varepsilon(r_1, r)\, \mathcal{G}^R_\varepsilon(r, r_2) = (\partial/\partial\varepsilon)\, \mathcal{G}^R_\varepsilon(r_1, r_2)$, and expressing $n(\vec{r})$ in terms of $\mathcal{G}^R_\varepsilon$, we find:

$$\delta\nu_H(\varepsilon) = \frac{2}{\pi^2 V_d} \operatorname{Re} \int dr_1 dr_2\, V(\vec{r}_1 - \vec{r}_2) \int_{-\varepsilon_F}^{0} d\varepsilon_1 \left[\mathcal{G}^R_{\varepsilon_1}(r_2, r_2) - \mathcal{G}^A_{\varepsilon_1}(r_2, r_2)\right] \frac{\partial}{\partial\varepsilon}\, \mathcal{G}^R_\varepsilon(r_1, r_1) \tag{87}$$

5. Interaction correction to DOS in the diffusive limit.

Instead of considering a cross-term of the type "impurity – Friedel one." as in Eq. (79) we could introduce $\mathcal{G}^R_\varepsilon(r_1, r_2)$ accounting for <u>all</u> the impurities, and then evaluate the first-order correction in V_H and V_{ex} (also evaluated with the ~~hep~~ help of $\mathcal{G}_\varepsilon(r_1, r_2)$, rather than free-fermion $G(\varepsilon, r_1, r_2)$ function):

$$\delta \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}) = \int dr_1\, \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}_1) V_H(\vec{r}_1) \mathcal{G}^R_\varepsilon(\vec{r}_1, \vec{r})$$
$$- \int d\vec{r}_1 d\vec{r}_2\, \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}_1) V_{ex}(\vec{r}_1, \vec{r}_2) \mathcal{G}^R_\varepsilon(r_2, r) \qquad (86)$$

We are interested in $\delta\nu(\varepsilon) = (1/V_d) \int d^d\vec{r}\, \delta\nu(\varepsilon, \vec{r})$. That allows us to employ identity

$$\int dr\, \mathcal{G}^R_\varepsilon(\vec{r}_2, \vec{r}) \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}_1) = \frac{\partial}{\partial\varepsilon} \mathcal{G}^R_\varepsilon(\vec{r}_2, \vec{r}_1) \qquad (87)$$

in averaging of $\mathrm{Im}(\delta \mathcal{G}^R_\varepsilon(\vec{r}, \vec{r}))$ of Eq. (86).

We concentrate now on the exchange contribution (the Hartree one is dealt with similarly). Expressing $V_{ex}(r_1, r_2)$ in terms of $\mathrm{Im}\int_{-\varepsilon_F}^0 d\varepsilon\, \mathcal{G}_\varepsilon(r_1, r_2)$ and using Eq. (87), we find

$$\delta\nu_{ex}(\varepsilon) = -\frac{2}{\pi^2 V_d} \mathrm{Re} \int_{-\varepsilon_F}^{0} d\varepsilon_1 \int d\vec{r}_1 d\vec{r}_2\, V(\vec{r}_1 - \vec{r}_2) \frac{\partial \mathcal{G}^R_\varepsilon(\vec{r}_2, \vec{r}_1)}{\partial\varepsilon}$$
$$\times \left[\mathcal{G}^R_{\varepsilon_1}(\vec{r}_1, \vec{r}_2) - \mathcal{G}^A_{\varepsilon_1}(\vec{r}_1, \vec{r}_2) \right] \qquad (88)$$

Clearly in the averaging the reducible part of $\langle (\partial G^R_\varepsilon/\partial\varepsilon)\,\mathrm{Im}\, G^R_\varepsilon \rangle$ yields zero, so only the diffuson part remains,

$$\frac{\langle \delta\nu_{ex}(\varepsilon)\rangle}{\nu_0} = \frac{1}{\pi}\,\mathrm{Re}\int_\varepsilon^\infty d\omega \cdot \frac{1}{V_d}\int d\vec r_1\, d\vec r_2\, V(\vec r_1-\vec r_2) \times \frac{\partial}{\partial\omega} D(\omega, \vec r_2-\vec r_1) \qquad (89)$$

Generalizable onto arbitrary $\varepsilon\tau/\hbar$; to describe crossover from quasi-ballistic to diffusive motion, use kinetic eq. for D

$$= \frac{1}{\pi}\,\mathrm{Re}\int_\varepsilon^\infty d\omega \int \frac{d^d\vec q}{(2\pi)^d}\, V(\vec q)\,\frac{\partial}{\partial\omega} D(\omega,\vec q); \quad d=1,2,3$$

In the case of long-range (Coulomb) potential

$$V(q) \to V_{scr}(q,\omega) = \frac{V(q)}{1+V(q)\Pi(q,\omega)} \quad (\mathrm{RPA}) \qquad (90)$$

with $\Pi(q,\omega) = \nu_0\,[1+i\omega D(\omega,q)]$ (91)

(dynamic screening)

In the case of finite-range potential in 2D,

$$\langle \delta\nu(\varepsilon)\rangle \propto -\Big(\underset{\uparrow\atop ex}{V(0)} - 2\underset{\uparrow\atop H}{\overline{V}}^{\,\text{Fermi surface}}\Big)\ln(\hbar/\varepsilon\tau) \qquad (92)$$

For the Coulomb potential in <u>2D</u> (Altshuler, Aronov, Lee 79, 80 - see refs. in the review quoted on p. 23)

$$\frac{\langle\delta\nu(\varepsilon)\rangle}{\nu_0} \propto -\frac{1}{E_F\tau}\ln\left(\frac{\varepsilon\tau}{\hbar}\right)\ln(\varepsilon/\varepsilon_0) \qquad (93)$$

with $\varepsilon_0 \sim D/r_D^2$.

① Corrections to conductivity in terms of Friedel oscillations: see Zala et. al. – PRB <u>64</u>, 214201 (2001).

② ZBA in tunneling experiment (metallic wire): F. Pierre et. al. PRL <u>86</u>, 1590 (2001)