# Potential scattering in metals and unconventional superconductors

## Strong potentials with finite range.

Kurt Scharnberg

I. Institut für Theoretische Physik, Universität Hamburg

# Contents

- Motivation
  - microwave conductivity
- Strong (resonant) scattering, (generalized) T-Matrix
  - single impurity,   local density of states LDOS
  - alloy model, (small concentration of impurities) selfenergies

# Contents

- Motivation
  - microwave conductivity
- Strong (resonant) scattering, (generalized) T-Matrix
  - single impurity,   local density of states LDOS
  - alloy model, (small concentration of impurities) selfenergies
- (Extended) scatterers in the Fermi surface restricted approximation: Problems and possible solutions.

# Contents

- Motivation
  - microwave conductivity
- Strong (resonant) scattering, (generalized) T-Matrix
  - single impurity,   local density of states LDOS
  - alloy model, (small concentration of impurities) selfenergies
- (Extended) scatterers in the Fermi surface restricted approximation: Problems and possible solutions.
- Results:
  - Full theory (NFE-Model) for normal metals
  - $\delta$-function scatterers and finite band width; graphene
- Summary

# Motivation

Impurities dominate low temperature (low frequency) properties of metals and superconductors. (spectral functions (ARPES), microwave conductivity, thermal conductivity.) Potential scattering leads to $T_c$-suppression in unconventional superconductors.

# Motivation

Impurities dominate low temperature (low frequency) properties of metals and superconductors. (spectral functions (ARPES), microwave conductivity, thermal conductivity.) Potential scattering leads to $T_c$-suppression in unconventional superconductors.

$\delta$-function potentials in 2D and 3D do not lead to scattering, unless uncontrolled approximations are made.

Many results based on these approximations have been published.

When the same uncontrolled approximations are applied to finite range potentials, results which are clearly unphysical follow.
The finite range, when correctly treated, will not only provide a scattering mechanism, it will affect the conductivity (no longer universal) and the $T_c$-suppression ($d$-wave pairing + $d$-wave scattering?)

# Motivation

Impurities dominate low temperature (low frequency) properties of metals and superconductors. (spectral functions (ARPES), microwave conductivity, thermal conductivity.) Potential scattering leads to $T_c$-suppression in unconventional superconductors.

$\delta$-function potentials in 2D and 3D do not lead to scattering, unless uncontrolled approximations are made.

Many results based on these approximations have been published.

When the same uncontrolled approximations are applied to finite range potentials, results which are clearly unphysical follow.
The finite range, when correctly treated, will not only provide a scattering mechanism, it will affect the conductivity (no longer universal) and the $T_c$-suppression ($d$-wave pairing + $d$-wave scattering?)

Variations in the Local Density of States (LDOS) near a defect, experimentally accessible through Scanning Tunneling Microscopy/Spectroscopy (STM/STS) provide information on the properties of the host system, as well as the defect.

# Microwave Absorption - Experimental Facts

**The dissipation, measured by $\sigma_1(\omega, T)$ or $R_s(\omega, T)$, at microwave frequencies and low temperatures is not well understood, even in the linear response regime:**

- **it is too high at very low T,**
- **it's temperature dependence is in conflict with any fairly straightforward semi-microscopic theory.**

**Real part of the in-plane conductivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ poses the biggest problems!**

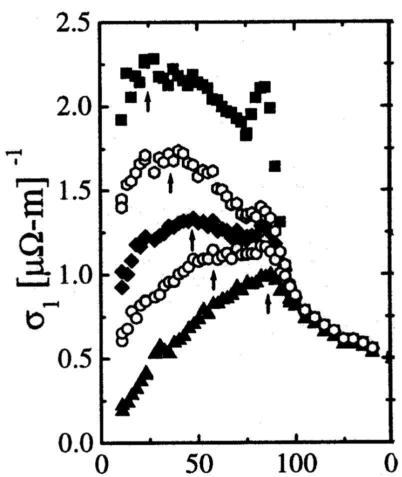
# *Microwave Absorption - Experimental Facts*

**The dissipation, measured by $\sigma_1(\omega, T)$ or $R_s(\omega, T)$, at microwave frequencies and low temperatures is not well understood, even in the linear response regime:**

- **it is too high at very low T,**
- **it's temperature dependence is in conflict with any fairly straightforward semi-microscopic theory.**

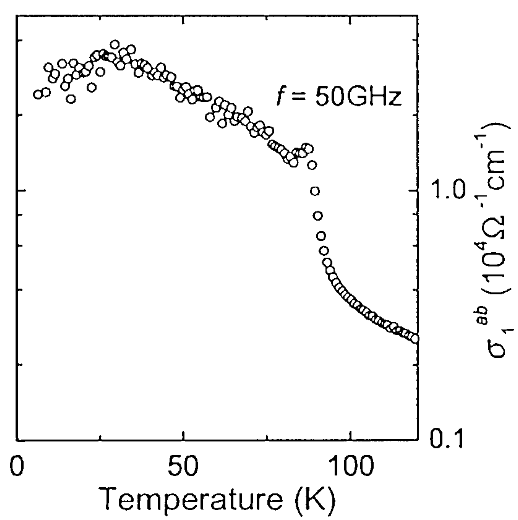
**Real part of the in-plane conductivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ poses the biggest problems!**

**Corson et al., PRL 85 (2000) 2569**



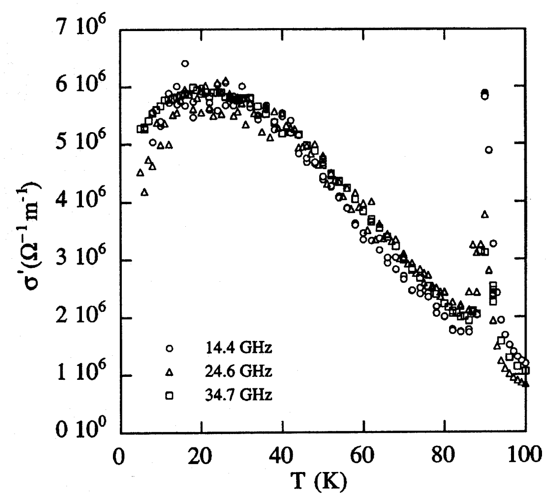

**$\sigma_1$ plotted versus temperature for 0.2, 0.3, 0.4, 0.6, and 0.8 THz as squares, octagons, diamonds, circles, and triangles, respectively.**
**At each frequency the arrows mark the temperature where $\sigma_1$ begins to decrease.**

**H. Kitano et al., J. Low Temp. Phys. 117 (1999) 1241**




**$\sigma_1$ plotted versus temperature for 50 GHz.**
**Note the logarithmic scale.**

**Shih-Fu Lee et al., PRL 77 (1996) 735**




**$\sigma_1$ plotted versus temperature for 14.4, 24.6, and 34.7 GHz**
**$\sigma_1$ is basically frequency independent in this frequency regime and exhibits a broad peak at VERY low temperature.**

# Microwave conductivity in terms of the two-fluid model

$$\sigma_1^{\mathrm{two-fl}}(\omega, T) = \frac{1}{\mu_0 \lambda_p^2} \frac{2\Gamma(\omega,T)}{4\Gamma^2(\omega,T)+\omega^2}\, \rho_n$$

**which relates $\sigma(\omega, T)$ to the normal fluid fraction $\rho_n = 1 - \rho_s$, the London penetration depth $\lambda_p$, and a frequency and temperature dependent scattering rate $\Gamma(\omega, T)$.**

**For $\sigma_1$ to be large, $\rho_n$ must remain finite (how large can $\rho_n$ be?) for low $T$.**
**This requires extremely anisotropic $s$-wave or unconventional superconductivity.**

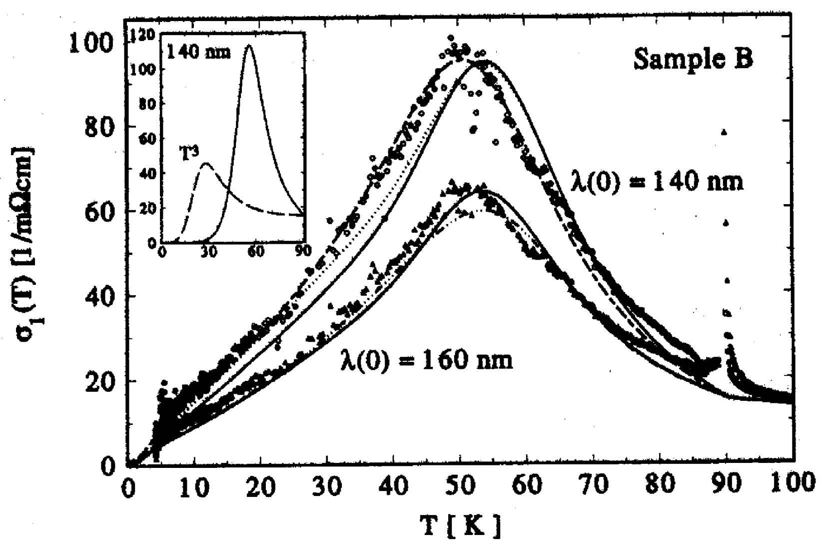
# Microwave conductivity in terms of the two-fluid model

$$\sigma_1^{\mathrm{two-fl}}(\omega, T) = \frac{1}{\mu_0 \lambda_p^2} \frac{2\Gamma(\omega,T)}{4\Gamma^2(\omega,T)+\omega^2}\,\rho_n$$

**which relates $\sigma(\omega, T)$ to the normal fluid fraction $\rho_n = 1 - \rho_s$, the London penetration depth $\lambda_p$, and a frequency and temperature dependent scattering rate $\Gamma(\omega, T)$.**

**For $\sigma_1$ to be large, $\rho_n$ must remain finite (how large can $\rho_n$ be?) for low $T$.**
**This requires extremely anisotropic $s$-wave or unconventional superconductivity.**

**Hensen et al., Phys. Rev. B 56 (1997) 6237**




**$\sigma_1(T)$ obtained from measurements of $R_s(T)$ on a high quality YBCO film at 87 GHz.**
**$\sigma_1(T)$ extracted from $R_s(T)$ depends strongly on the choice of $\lambda(0)$, which is much more difficult to measure accurately than the change of penetration depth with temperature.**

**Furthermore, $\Gamma(T)$ has to decrease as $T \to 0$. But this increases $\sigma_1$ only as long as $2\Gamma > \omega$.**

**Defect scattering needs to be taken into account!**

**When $\rho_s(T)$ is determined from measurements of the penetration depth, the linear $T$-dependence of $\sigma_1$ observed in the cleanest samples requires $\Gamma$ to be temperature independent.**
**THERE IS A PROBLEM!**

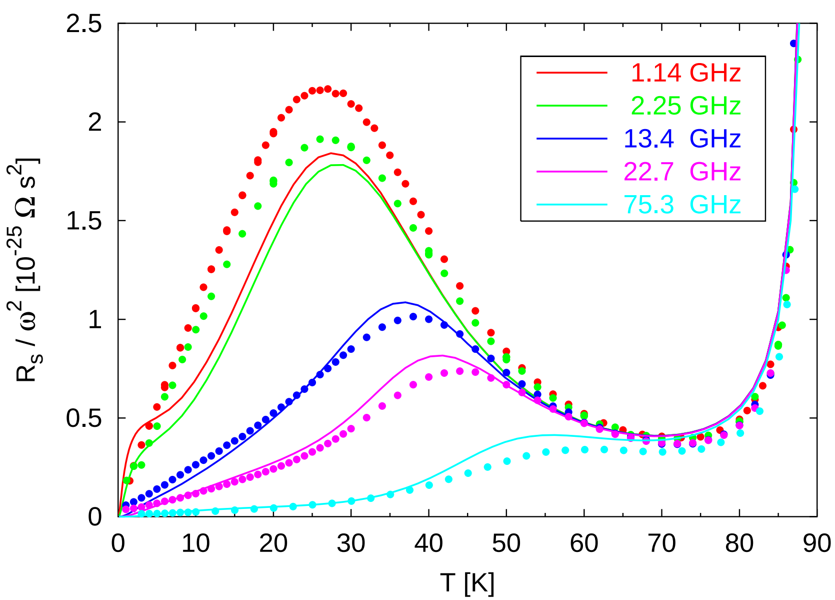
# Measurements on $YBa_2Cu_3O_{7-\delta}$ single crystals, Calculations for point-like defects of arbitrary strength.

**Measurements of the surface resistance $R_s$ as function of temperature at a range of microwave frequency on high quality $YBa_2Cu_3O_{7-\delta}$ single crystals from $BaZrO_3$ crucibles. Since extracting the conductivity requires assumptions with respect to the penetration depth, we have fitted $R_s$ itself.**

# Measurements on $YBa_2Cu_3O_{7-\delta}$ single crystals, Calculations for point-like defects of arbitrary strength.

**Measurements of the surface resistance $R_s$ as function of temperature at a range of microwave frequency on high quality $YBa_2Cu_3O_{7-\delta}$ single crystals from $BaZrO_3$ crucibles. Since extracting the conductivity requires assumptions with respect to the penetration depth, we have fitted $R_s$ itself.**

**Exp:Hosseini et al., Phys. Rev. B 60(1999)1349**
**Theory: Rieck et al., J. Low Temp. Phys. 117 (1999) 1295**




**A very small elastic scattering rate $\Gamma_N^{el} = 0.015\,meV$ and a scattering phase shift $\delta_N = 0.44\pi$ have been deduced from the low temperature data. At higher temperatures a phenomenological temperature dependent scattering rate has been introduced.**

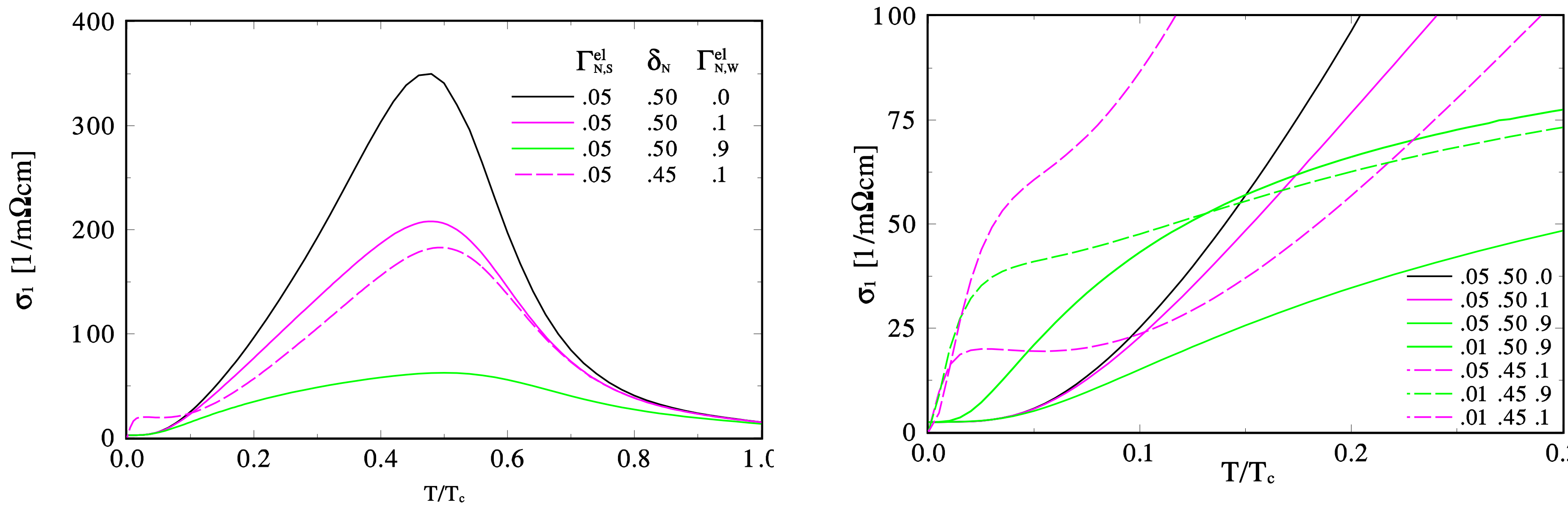
**The peak heights can only be reproduced if the $T^3$–dependence of the inelastic scattering rate derived from spin fluctuation exchange is absent from the scattering rate relevant for electrical transport. (Umklapp processes!?)**

**A better fit to the peaks observed at the two lowest frequencies could be obtained by changing $\Gamma_N^{el}$ and $\delta_N$. Agreement at higher frequencies then deteriorates, but this only indicates that the T–dependent inelastic scattering should also be frequency dependent.**

**Note the strange behaviour of the fit at low temperatures and low frequencies!**

# Strong and Weak Scatterers

MSCATIIB May 18, 2004 7:01:29 PM




**Combined effect of strong and weak point-like scatterers on the real part of the conductivity of a $d$-wave superconductor at 4.13GHz. The first and third column of the legend contain the normal state elastic scattering rates in meV for strong (S) and weak (W) scatterers. The center column gives the phase shift in units of $\pi$. Weak scattering implies: $\delta_N = 0.01\pi$.**

SUMMARY: Weak point-like scatterers have no effect on the real part of the conductivity at low temperatures, but drastically reduce the peak at intermediate temperatures.

**Rôle of forward scattering?**

# Strong Scattering

Effects of strongly scattering impurities are described by a (generalized) $T$-matrix, which is to be determined from a (2D) Fredholm integral equation of the 2nd kind.

It cannot be solved by iteration (Born series diverges! Use wavelets)

For isotropic systems a Fourier expansion with respect to angle ist possible. This leads to sets of one-dimensional integral equations which we have solved!

# Strong Scattering

Effects of strongly scattering impurities are described by a (generalized) $T$-matrix, which is to be determined from a (2D) Fredholm integral equation of the 2nd kind.

It cannot be solved by iteration (Born series diverges! Use wavelets)

For isotropic systems a Fourier expansion with respect to angle ist possible. This leads to sets of one-dimensional integral equations which we have solved!

As input, some scattering potential is required. (Model: Gaussian, hard disk)

- Single impurity: Calculate the LDOS and, in the case of superconductors, the spatial modulation of the Order Parameter.
- For an ensemble of independent scattering centers, averaging with respect to defect positions makes the system translationally invariant. The (normal and anomalous) selfenergies have to be calculated selfconsistently.

# Equation of motion for the Green functions

**Singlet pairing:**

$$\begin{aligned}
\left[i\omega_n + \frac{1}{2m}\vec{\nabla}^2 + \mu + V(\vec{r})\right] G_{\uparrow\uparrow}(\vec{r},\vec{r}',i\omega_n) - \int d^2\rho\, \Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho})\, \bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}',\omega_n) &= \delta(\vec{r}-\vec{r}') \\
\int d^2\rho\, \bar{\Delta}_{\downarrow\uparrow}(\vec{r},\vec{\rho})\, G_{\uparrow\uparrow}(\vec{\rho},\vec{r}',\omega_n) - \left[i\omega_n - \frac{1}{2m}\vec{\nabla}^2 - \mu - V(\vec{r})\right] \bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}',\omega_n) &= 0
\end{aligned}$$

# Equation of motion for the Green functions

Singlet pairing:

$$\left[i\omega_n + \frac{1}{2m}\vec{\nabla}^2 + \mu + V(\vec{r})\right] G_{\uparrow\uparrow}(\vec{r},\vec{r}\,',i\omega_n) - \int d^2\rho\, \Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho})\, \bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n) = \delta(\vec{r}-\vec{r}\,')$$

$$\int d^2\rho\, \bar{\Delta}_{\downarrow\uparrow}(\vec{r},\vec{\rho})\, G_{\uparrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n) - \left[i\omega_n - \frac{1}{2m}\vec{\nabla}^2 - \mu - V(\vec{r})\right] \bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n) = 0$$

BCS Theory: $\Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho}) = \Delta_{\uparrow\downarrow}(\vec{r})\,\delta(\vec{r}-\vec{\rho})$ (cf. Fetter)

Translationally invariant system ($V(\vec{r})$ absent): $\Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho}) = \Delta_{\uparrow\downarrow}(\vec{r}-\vec{\rho})$
Then the equation of motion can be solved by Fourier transformation.

The result is a set of BCS-like Green functions with $\Delta$ replaced by $\Delta(\vec{k})$

# *Equation of motion for the Green functions*

Singlet pairing:

$$\begin{aligned}\left[i\omega_n+\frac{1}{2m}\vec{\nabla}^2+\mu+V(\vec{r})\right]G_{\uparrow\uparrow}(\vec{r},\vec{r}\,',i\omega_n)-\int d^2\rho\,\Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho})\,\bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n) &= \delta(\vec{r}-\vec{r}\,')\\ \int d^2\rho\,\bar{\Delta}_{\downarrow\uparrow}(\vec{r},\vec{\rho})\,G_{\uparrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n)-\left[i\omega_n-\frac{1}{2m}\vec{\nabla}^2-\mu-V(\vec{r})\right]\bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n) &= 0\end{aligned}$$

BCS Theory: $\Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho}) = \Delta_{\uparrow\downarrow}(\vec{r})\,\delta(\vec{r}-\vec{\rho})$ (cf. Fetter)

Translationally invariant system ($V(\vec{r})$ absent): $\Delta_{\uparrow\downarrow}(\vec{r},\vec{\rho}) = \Delta_{\uparrow\downarrow}(\vec{r}-\vec{\rho})$
Then the equation of motion can be solved by Fourier transformation.
The result is a set of BCS-like Green functions with $\Delta$ replaced by $\Delta(\vec{k})$

With $V(\vec{r})$ present, $\bar{F}_{\downarrow\uparrow}(\vec{\rho},\vec{r}\,',\omega_n)$ is modified and hence, via the selfconsistency equation, also $\bar{\Delta}_{\downarrow\uparrow}(\vec{r},\vec{\rho})$. Separation of relative and center of mass coordinates is a problem when one is interested in Friedel oscillations of a $d$-wave order parameter near an impurity!

## Equation of motion for the Green functions in integral form:

(without the order parameter fluctuation)

$$\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}^0(\boldsymbol{r}-\boldsymbol{r}';\omega) + \int d^2\rho\, \hat{G}^0(\boldsymbol{r}-\boldsymbol{\rho};\omega)\, V(\boldsymbol{\rho})\hat{\sigma}_3\, \hat{G}(\boldsymbol{\rho},\boldsymbol{r}';\omega)$$

Given $\hat{G}^0(\mathbf{r}-\mathbf{r}';\omega)$ and $V(\boldsymbol{\rho})$, this could be solved directly to give the

LDOS $\quad N(\mathbf{r}) = -\frac{1}{\pi}\mathcal{I}m\, G_{11}(\boldsymbol{r},\boldsymbol{r};\omega) \qquad$ (or $\rho(\mathbf{r})$; March, Angilella)

## Equation of motion for the Green functions in integral form:

(without the order parameter fluctuation)

$$\hat{G}(\mathbf{r},\mathbf{r}';\omega)=\hat{G}^0(\boldsymbol{r}-\boldsymbol{r'};\omega)+\int d^2\rho\,\hat{G}^0(\boldsymbol{r}-\boldsymbol{\rho};\omega)\,V(\boldsymbol{\rho})\hat{\sigma}_3\,\hat{G}(\boldsymbol{\rho},\boldsymbol{r'};\omega)$$

Given $\hat{G}^0(\mathbf{r}-\mathbf{r}';\omega)$ and $V(\boldsymbol{\rho})$, this could be solved directly to give the

LDOS $\quad N(\mathbf{r}) = -\dfrac{1}{\pi}\mathcal{I}m\,G_{11}(\boldsymbol{r},\boldsymbol{r};\omega)$ $\qquad$ (or $\rho(\mathbf{r})$; March, Angilella)

For $V(\boldsymbol{\rho}) = V\,\delta(\boldsymbol{\rho})$, the solution is trivial:

$$\begin{aligned}\hat{G}(\boldsymbol{r},\boldsymbol{r'};\omega) &= \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'};\omega)+\\ &\quad +V\,\hat{G}^0(\boldsymbol{r};\omega)\,\hat{\sigma}_3\left(\hat{\sigma}_0-V\,\hat{G}^0(0;\omega)\,\hat{\sigma}_3\right)^{-1}\hat{G}^0(-\mathbf{r}';\omega)\end{aligned}$$

In 2D $\hat{G}^0(0;\omega)=\int\frac{d^Dk}{(2\pi)^D}\,\hat{G}^0(\boldsymbol{k};\omega_n)$ diverges as $\ln r$ as $r\to 0$ so that the second term vanishes, unless the band width is finite!

**This approach was used to calculate the LDOS of graphene.**

# Generalized $T$-Matrix

Introducing the generalized $T$-Matrix

$$\hat{T}(\boldsymbol{k},\boldsymbol{k'};\omega) = V(\boldsymbol{k}-\boldsymbol{k'})\hat{\sigma}_3 + \int\frac{d^2p}{(2\pi)^2}V(\boldsymbol{k}-\boldsymbol{p})\,\hat{\sigma}_3\,\hat{G}^0(\boldsymbol{p},\omega)\,\hat{T}(\boldsymbol{p},\boldsymbol{k'};\omega)\,,$$

the equation of motion for the Green functions can be recast in the form

$$\begin{aligned}\hat{G}(\boldsymbol{r},\boldsymbol{r'},\omega) &= \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'},\omega) + \\ &+ \int\frac{d^2k}{(2\pi)^2}\int\frac{d^2k'}{(2\pi)^2}e^{i\boldsymbol{kr}}\,\hat{G}^0(\boldsymbol{k},\omega)\hat{T}(\boldsymbol{k},\boldsymbol{k'};\omega)\hat{G}^0(\boldsymbol{k'},\omega)\,e^{-i\boldsymbol{k'r'}}.\end{aligned}$$

The $T$-matrix known from scattering theory is $\hat{T}(\mathbf{k},\mathbf{k}') = \hat{T}(\mathbf{k},\mathbf{k}';\epsilon(\mathbf{k}'))$

# *Generalized* $T$*-Matrix*

Introducing the generalized $T$-Matrix

$$\hat{T}(\boldsymbol{k},\boldsymbol{k'};\omega) = V(\boldsymbol{k}-\boldsymbol{k'})\hat{\sigma}_3 + \int\frac{d^2p}{(2\pi)^2}V(\boldsymbol{k}-\boldsymbol{p})\,\hat{\sigma}_3\,\hat{G}^0(\boldsymbol{p},\omega)\,\hat{T}(\boldsymbol{p},\boldsymbol{k'};\omega)\,,$$

the equation of motion for the Green functions can be recast in the form

$$\begin{aligned}\hat{G}(\boldsymbol{r},\boldsymbol{r'},\omega) &= \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'},\omega) + \\ &+ \int\frac{d^2k}{(2\pi)^2}\int\frac{d^2k'}{(2\pi)^2}e^{i\boldsymbol{k}\boldsymbol{r}}\,\hat{G}^0(\boldsymbol{k},\omega)\hat{T}(\boldsymbol{k},\boldsymbol{k'};\omega)\hat{G}^0(\boldsymbol{k'},\omega)\,e^{-i\boldsymbol{k'}\boldsymbol{r'}}.\end{aligned}$$

The $T$-matrix known from scattering theory is $\hat{T}(\mathbf{k},\mathbf{k}') = \hat{T}(\mathbf{k},\mathbf{k}';\epsilon(\mathbf{k}'))$

With $V(\boldsymbol{\rho})$ representing a single defect, we used these two equations for an isotropic system to calculate the LDOS.

With $V(\boldsymbol{\rho})$ representing an ensemble of defects, taking a configuration average leads to a translationally invariant Green function

$$\hat{G}(\boldsymbol{r},\boldsymbol{r'},\omega) = \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'},\omega)+\int\frac{d^2k}{(2\pi)^2}e^{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r'})}\,\hat{G}^0(\boldsymbol{k},\omega)\hat{\Sigma}(\boldsymbol{k},\omega)\hat{G}(\boldsymbol{k},\omega)$$

where the selfenergy $\hat{\Sigma}(\mathbf{k},\omega) = n_{\mathrm{imp}}\hat{t}(\mathbf{k},\mathbf{k},\omega)$ has been introduced.

With $V(\boldsymbol{\rho})$ representing an ensemble of defects, taking a configuration average leads to a translationally invariant Green function

$$\hat{G}(\boldsymbol{r},\boldsymbol{r'},\omega) = \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'},\omega)+\int\frac{d^2k}{(2\pi)^2}e^{i\boldsymbol{k(r-r')}}\,\hat{G}^0(\boldsymbol{k},\omega)\hat{\Sigma}(\boldsymbol{k},\omega)\hat{G}(\boldsymbol{k},\omega)$$

where the selfenergy $\hat{\Sigma}(\mathbf{k},\omega) = n_{\text{imp}}\hat{t}(\mathbf{k},\mathbf{k},\omega)$ has been introduced.
The solution for the Green function is straightforward

$$\hat{G}(\boldsymbol{k},\omega) = \left[\omega\hat{\sigma}_0 - \varepsilon(\boldsymbol{k})\hat{\sigma}_3 - \Delta(\boldsymbol{k})\hat{\sigma}_1 - \hat{\Sigma}(\boldsymbol{k},\omega)\right]^{-1}$$

$$\hat{t}(\boldsymbol{k},\boldsymbol{k'};\omega) = v(\boldsymbol{k}-\boldsymbol{k'})\hat{\sigma}_3 + \int\frac{d^2p}{(2\pi)^2}v(\boldsymbol{k}-\boldsymbol{p})\,\hat{\sigma}_3\,\hat{G}(\boldsymbol{p},\omega)\,\hat{t}(\boldsymbol{p},\boldsymbol{k'};\omega)$$

**$\hat{t}$ is the $T$-matrix for a single defect,** to be calculated selfconsistently!

$\hat{G}$ and $\hat{t}$ are expanded in terms of Pauli matrices.

$$t^0 = \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^3 + \frac{\varepsilon}{D} t^0 - \frac{\Delta}{D} t^2\right]$$

$$t^1 = \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^2 + \frac{\varepsilon}{D} t^1 - \frac{\Delta}{D} t^3\right]$$

$$t^2 = \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^1 + \frac{\varepsilon}{D} t^2 + \frac{\Delta}{D} t^0\right]$$

$$t^3 = v + \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^0 + \frac{\varepsilon}{D} t^3 + \frac{\Delta}{D} t^1\right]$$

$$D = \omega^2 - \varepsilon^2(p) - \Delta^2(p)$$

$$
\begin{aligned}
t^0 &= \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^3 + \frac{\varepsilon}{D} t^0 - \frac{\Delta}{D} t^2\right] \\
t^1 &= \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^2 + \frac{\varepsilon}{D} t^1 - \frac{\Delta}{D} t^3\right] \\
t^2 &= \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^1 + \frac{\varepsilon}{D} t^2 + \frac{\Delta}{D} t^0\right] \\
t^3 &= v + \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^0 + \frac{\varepsilon}{D} t^3 + \frac{\Delta}{D} t^1\right]
\end{aligned}
$$

$$D = \omega^2 - \varepsilon^2(p) - \Delta^2(p)$$

**Quasiclassical Approximation: perform the energy integration assuming particle-hole symmetry. Terms marked in red vanish!**

$$
\begin{aligned}
t^0 &= \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^3 + \frac{\varepsilon}{D} t^0 - \frac{\Delta}{D} t^2\right] \\
t^1 &= \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^2 + \frac{\varepsilon}{D} t^1 - \frac{\Delta}{D} t^3\right] \\
t^2 &= \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^1 + \frac{\varepsilon}{D} t^2 + \frac{\Delta}{D} t^0\right] \\
t^3 &= v + \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^0 + \frac{\varepsilon}{D} t^3 + \frac{\Delta}{D} t^1\right]
\end{aligned}
$$

$$D = \omega^2 - \varepsilon^2(p) - \Delta^2(p)$$

Quasiclassical Approximation: perform the energy integration assuming particle-hole symmetry. Terms marked in red vanish!

This approximation is justified (Eilenberger, Larkin, Ovchinnikov) with the argument that only differences between the superconducting and the normal state need to be considered. Here, subtracting the corresponding normal state equations does not improve the convergence of the $\varepsilon$-integral.

## Fermi surface restricted approximation

**For a circular Fermi surface the previous set of equations reduces to**

$$t^0(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^3(\psi,\phi) - g^1(\psi)\, t^2(\psi,\phi)\right.$$

$$t^1(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^2(\psi,\phi) - g^1(\psi)\, t^3(\psi,\phi)\right.$$

$$t^2(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^1(\psi,\phi) + g^1(\psi)\, t^0(\psi,\phi)\right.$$

$$t^3(\varphi,\phi) = v(\varphi-\phi) + \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0\, t^0(\psi,\phi) + g^1\, t^1(\psi,\phi\right.$$

## Fermi surface restricted approximation

**For a circular Fermi surface the previous set of equations reduces to**

$$t^0(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^3(\psi,\phi) - g^1(\psi)\, t^2(\psi,\phi)\right.$$

$$t^1(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^2(\psi,\phi) - g^1(\psi)\, t^3(\psi,\phi)\right.$$

$$t^2(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^1(\psi,\phi) + g^1(\psi)\, t^0(\psi,\phi)\right.$$

$$t^3(\varphi,\phi) = v(\varphi-\phi) + \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0\, t^0(\psi,\phi) + g^1\, t^1(\psi,\phi\right.$$

$g^0(\psi;\omega)$ and $g^1(\psi;\omega)$ are the energy integrated Green functions.

$g^0$ and $g^1$ are independent of $t^3(\psi,\psi)$ and $g^3$ vanishes.

## Fermi surface restricted approximation

**For a circular Fermi surface the previous set of equations reduces to**

$$t^0(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^3(\psi,\phi) - g^1(\psi)\, t^2(\psi,\phi)\right.$$

$$t^1(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^2(\psi,\phi) - g^1(\psi)\, t^3(\psi,\phi)\right.$$

$$t^2(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^1(\psi,\phi) + g^1(\psi)\, t^0(\psi,\phi)\right.$$

$$t^3(\varphi,\phi) = v(\varphi-\phi) + \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0\, t^0(\psi,\phi) + g^1\, t^1(\psi,\phi\right.$$

$g^0(\psi;\omega)$ and $g^1(\psi;\omega)$ are the energy integrated Green functions.

$g^0$ and $g^1$ are independent of $t^3(\psi,\psi)$ and $g^3$ vanishes.

All four components $t^\ell(\varphi,\phi)$ are required for the calculation of $\Sigma_{0,1}$.

# Fermi surface restricted approximation

## $\delta$-function scatterers.

$v = v_0$ is independent of angle and so are the $t^\ell$.

Then one has to average $g^1(\psi)$, which gives zero
FOR UNCONVENTIONAL SUPERCONDUCTORS
and hence $t^1 = t^2 = 0$.

# Fermi surface restricted approximation

## $\delta$-function scatterers.

$v = v_0$ is independent of angle and so are the $t^\ell$.

Then one has to average $g^1(\psi)$, which gives zero
FOR UNCONVENTIONAL SUPERCONDUCTORS
and hence $t^1 = t^2 = 0$. Final results:

$$t^0 = \frac{\pi N_F v_0^2 < g^0 >}{1 - (\pi N_F v_0)^2 < g^0 >^2}, \qquad t^3 = \frac{v_0}{1 - (\pi N_F v_0)^2 < g^0 >^2}$$

## Fermi surface restricted approximation

$\delta$-function scatterers.

$v = v_0$ is independent of angle and so are the $t^\ell$.

Then one has to average $g^1(\psi)$, which gives zero

FOR UNCONVENTIONAL SUPERCONDUCTORS

and hence $t^1 = t^2 = 0$. Final results:

$$t^0 = \frac{\pi N_F v_0^2 < g^0 >}{1 - (\pi N_F v_0)^2 < g^0 >^2}, \qquad t^3 = \frac{v_0}{1 - (\pi N_F v_0)^2 < g^0 >^2}$$

**Standard results, no problems!**

# Fermi surface restricted approximation

## $\delta$-function scatterers.

$v = v_0$ is independent of angle and so are the $t^\ell$.

Then one has to average $g^1(\psi)$, which gives zero

FOR UNCONVENTIONAL SUPERCONDUCTORS

and hence $t^1 = t^2 = 0$. Final results:

$$t^0 = \frac{\pi N_F v_0^2 < g^0 >}{1 - (\pi N_F v_0)^2 < g^0 >^2}, \qquad t^3 = \frac{v_0}{1 - (\pi N_F v_0)^2 < g^0 >^2}$$

## Standard results, no problems!

**Note some anomalies, however: $t^3$vanishes for $v_0 \to \infty$.**

**In this approximation, $t^3$has now effect on single particle properties.**

**$t^3$with $v_0$very large but finite was essential in obtaining a microwave conductivity bearing some similarity with experimental results on YBCO at low temperatures.**

## Fermi surface restricted approximation

**Solution of**

$$t^0(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^3(\psi,\phi) - g^1(\psi)\, t^2(\psi,\phi)\right] \;\mathrm{e}$$

**Solution of**

$$t^0(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^3(\psi,\phi) - g^1(\psi)\, t^2(\psi,\phi)\right] \text{e}$$

The potential $v$ is an even function of the angle $\varphi$ between $k_F$ and $k'_F$, which can be expanded as

$$v(\varphi) = v_0 \sum_{k=-\infty}^{+\infty} u_k\, e^{ik\varphi} \quad \text{with} \quad u_0 = 1$$

The $u_k$'s could be treated as parameters or could be calculated from some model potential in real space (hard disk, Gaussian, ...)

## Fermi surface restricted approximation

**Solution of**

$$t^0(\varphi,\phi) = \pi N_F \int_0^{2\pi} \frac{d\psi}{2\pi} v(\varphi-\psi)\left[g^0(\psi)\, t^3(\psi,\phi) - g^1(\psi)\, t^2(\psi,\phi)\right]$$

The potential $v$ is an even function of the angle $\varphi$ between $k_F$ and $k'_F$, which can be expanded as

$$v(\varphi) = v_0 \sum_{k=-\infty}^{+\infty} u_k\, e^{ik\varphi} \quad \text{with} \quad u_0 = 1$$

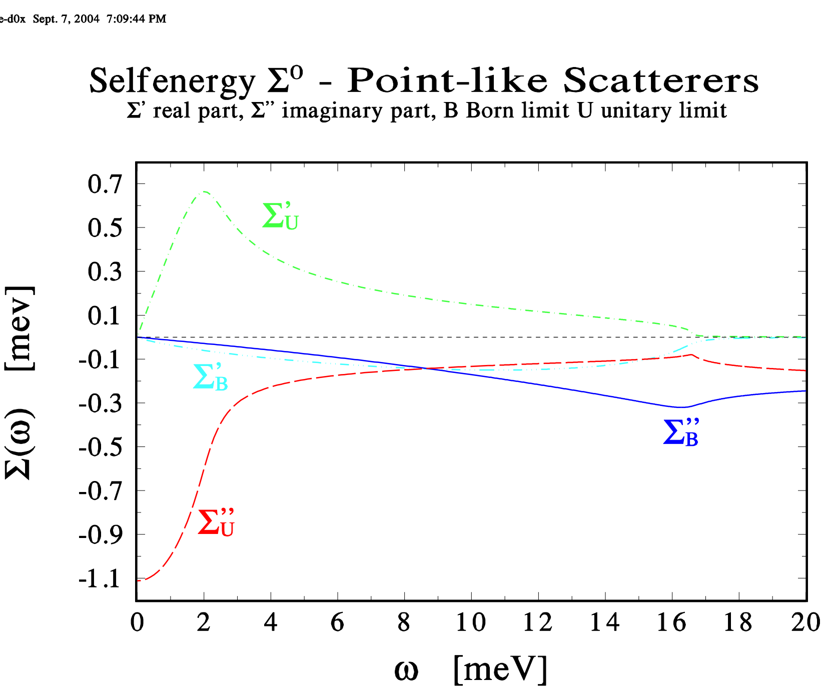
The $u_k$'s could be treated as parameters or could be calculated from some model potential in real space (hard disk, Gaussian, . . . )

The resulting system of coupled linear equations is solved, which gives $\hat{\Sigma}$, $\hat{G}$ and hence all single particle properties.

# Selfenergy $\Sigma^0$ for point-like scatterers

**The parameters introduced so far are combined in the following way:**

$$\pi N_F v_0 = \tan\delta_0\,, \qquad c = \cot\delta_0\,, \qquad \Gamma_{\rm N}^{\rm el} = \frac{n_{\rm imp}}{\pi N_F}\,\sin^2\delta_0$$




**For point-like scatterers $\Sigma^1 = 0$ and $\Sigma^0$ is independent of angle (momentum).**

**U: near unitary limit $\delta_0 = 0.49\pi$, $c = 0.03$,**
**B: near Born limit $\delta_0 = 0.10\pi$, $c = 3.1$**

**As is well-known: $\Sigma_B^{\prime\prime} \ll \Sigma_U^{\prime\prime}$ for $\omega \to 0$.**

**For elevated frequencies one finds $\Sigma_U^{\prime\prime} \leq \Sigma_B^{\prime\prime}$**

**For this reason, weak scatterers remove the peak in the microwave surface resistance at intermediate temperatures, without affecting the low temperature behavior.**
**(C.T. Rieck and K. Scharnberg: in *New Trends in Superconductivity*, NATO Science Series II, Vol. 67, J.F. Annett and S. Kruchinin (eds.), p.39)**

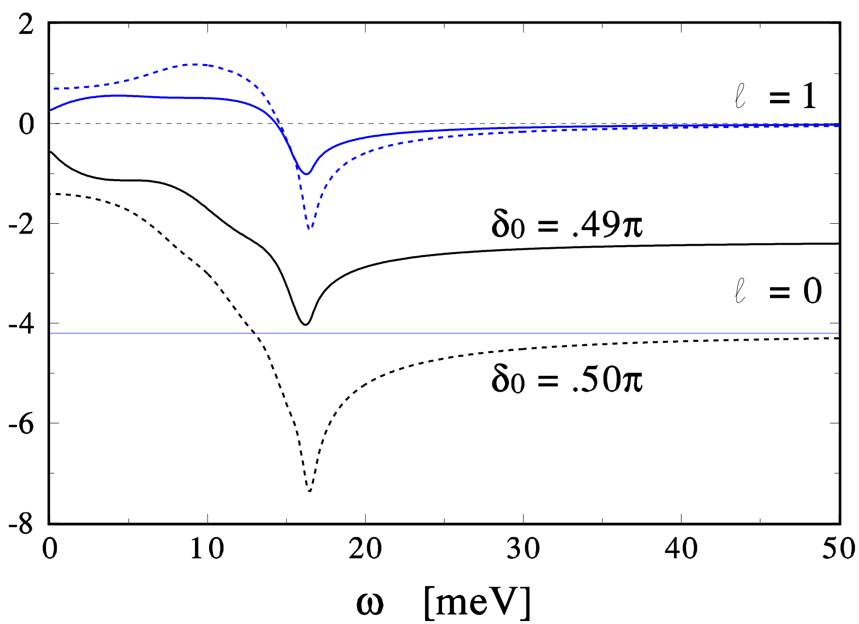
**For $\omega \to \infty$, $\Sigma_B^{\prime\prime}$ and $\Sigma_U^{\prime\prime}$ tend to $\Gamma_{\rm N}^{\rm el}$, choosen to be $0.2$ meV in these calculations.**

# *Selfenergy $\Sigma^0$ for Gaussian potential, limiting behavior*

**For $\omega \gg \Delta_{\max}$, (OP-Amplitude), $\Sigma^{0\ell}$ reduces to the normal state result:**

$$\Sigma^{00} = -i\,\Gamma_{\rm N}^{\rm el} \sum_{m=-M}^{M} \frac{u_m^2}{\cos^2\delta_0 + \sin^2\delta_0\, u_m^2}$$

9, 2004 9:57:51 PM




**Unitary limit:**

$$\Sigma^{00}(\delta_0 = 0.5\pi) = -i\,\Gamma_{\rm N}^{\rm el}(1+2M)\,.$$

**The limiting value in the Figure is $4.2$ meV since we have chosen $M = 10$.**

**There is a problem here with the Fermi surface restricted approach!.**

**For $\delta_0 = 0.49\pi$, the contribution from terms $m > 7$ is negligible. The limiting value is much larger, though, than for point-like scatterers.**

$\lim_{\omega\to\infty} \Sigma^{0\ell}$ with $\ell \neq 0$ vanishes,
because the normal state has been assumed to be isotropic.

# Full Theory for NFE model

$$t^3 = v + \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^0 + \frac{\varepsilon}{D} t^3 + \frac{\Delta}{D} t^1\right] \quad etc.$$

$$D(p,\psi) = \omega^2 - \varepsilon^2(p) - \Delta^2(p)\cos^2 2\psi$$

# Full Theory for NFE model

$$t^3 = v + \int \frac{d^2p}{(2\pi)^2}\, v \left[\frac{\omega}{D} t^0 + \frac{\varepsilon}{D} t^3 + \frac{\Delta}{D} t^1\right] \quad etc.$$

$$D(p,\psi) = \omega^2 - \varepsilon^2(p) - \Delta^2(p)\cos^2 2\psi$$

$$t^3(k,k',\phi,\phi') = V(k,k',\cos(\phi-\phi')) + \int_0^\infty \frac{dp\,p}{2\pi} \int_0^{2\pi} \frac{d\psi}{2\pi} V(k,p,\cos(\phi-\psi$$

$$\left[\frac{\omega}{D}\, t^0(p,k',\psi,\phi') + \frac{\varepsilon(p)}{D}\, t^3(p,k',\psi,\phi') + \frac{\Delta(p)\cos 2\psi}{D}\, t^1(p,k',\psi,\phi')\right]$$

**Expand in Fourierseries with respect to angle $\rightarrow$ System of coupled 1D integral equations, because the $d$-wave OP breaks rotational invariance.**
**In the non-selfconsistent case the $\psi$-integral can bre done analytically for all Fourier coefficients.**

# Model

**The potential $v$ is an even function of the angle $\varphi$ between $k_F$ and $k'_F$, which can be expanded as**

$$v(\varphi) = v_0 \sum_{k=-\infty}^{+\infty} u_k \, e^{ik\varphi} \quad \text{with} \quad u_0 = 1$$

**The $u_k$ could be varied at will!**

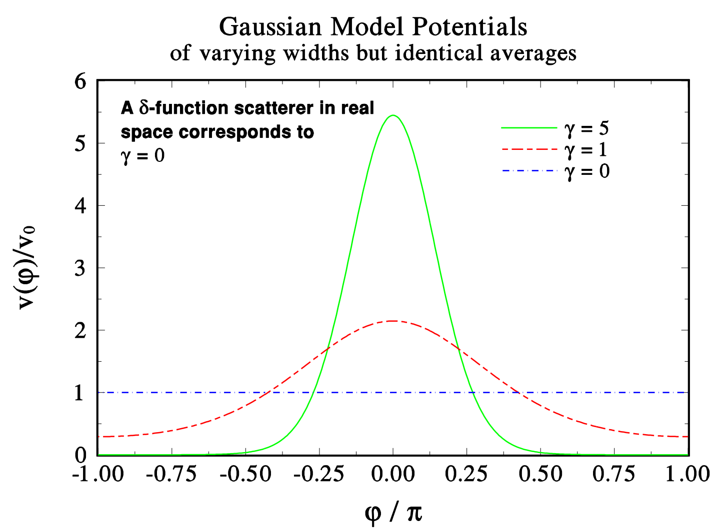
# Model

The potential $v$ is an even function of the angle $\varphi$ between $k_F$ and $k'_F$, which can be expanded as

$$v(\varphi) = v_0 \sum_{k=-\infty}^{+\infty} u_k \, e^{ik\varphi} \quad \text{with} \quad u_0 = 1$$

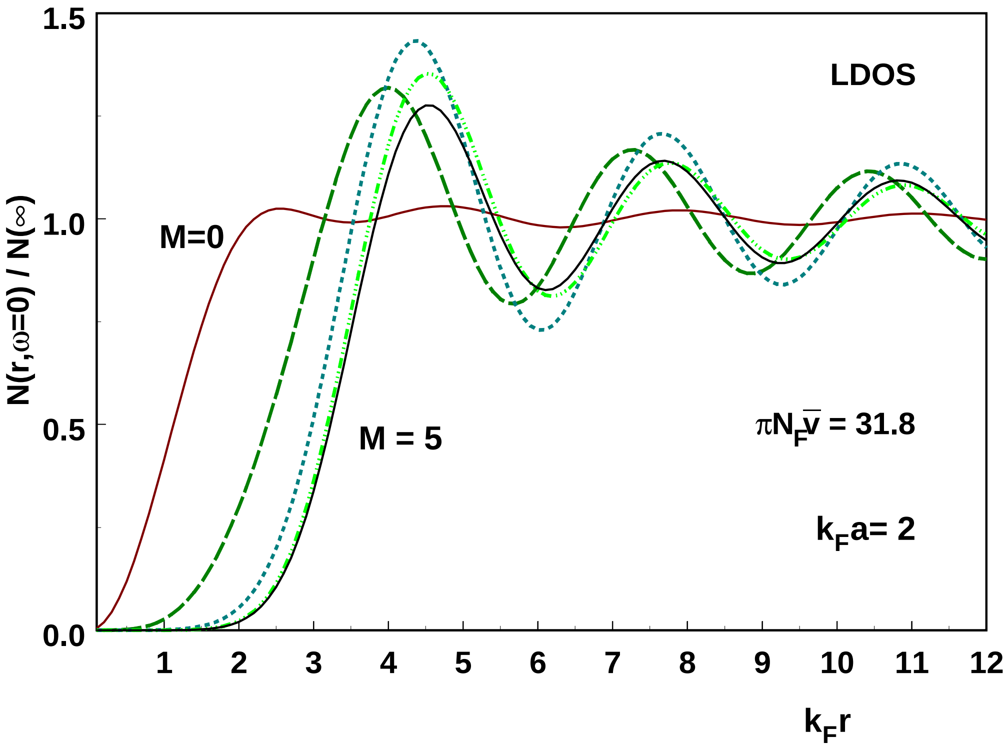
The $u_k$ could be varied at will!

As a specific model, which emphasizes forward scattering we consider a Gaussian $v(\varphi) = v_0 \frac{1}{I_0(\gamma)} e^{\gamma \cos \varphi}$ for which $u_k(\gamma) = I_k(\gamma)/I_0(\gamma)$




| $k$ | 1 (p) | 2 (d) | 3 (f) | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| $u_k(5)$ | 0.8934 | 0.6427 | 0.3793 | 0.1875 | 0.0792 | 0.0291 |
| $u_k(1)$ | 0.4463 | 0.1074 | 0.0174 | 0.0024 | 0.0002 | $< 10^{-4}$ |

# Full Theory: Normal State Results - LDOS




**Strong repulsive Gaussian scattering potential with fairly large range (compared to the Fermi wavelength)**

**Convergence of the Fourier series.**

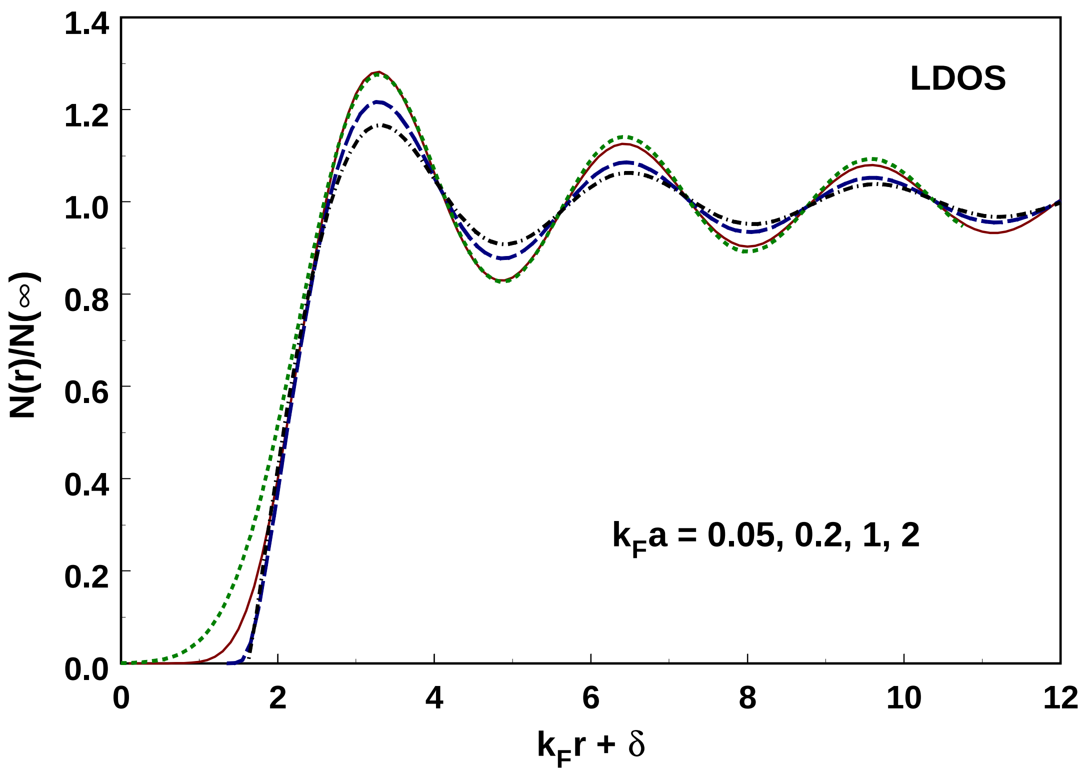
**The Friedel oscillations fall off as $r^{-1}$ in two dimensions.**

**Their amplitudes are much larger in 2D than in 3D!**

# Results - LDOS

**Comparison of strong Gaussian scatterers with different ranges.**

Spatial average $\bar{v}$ is kept constant!



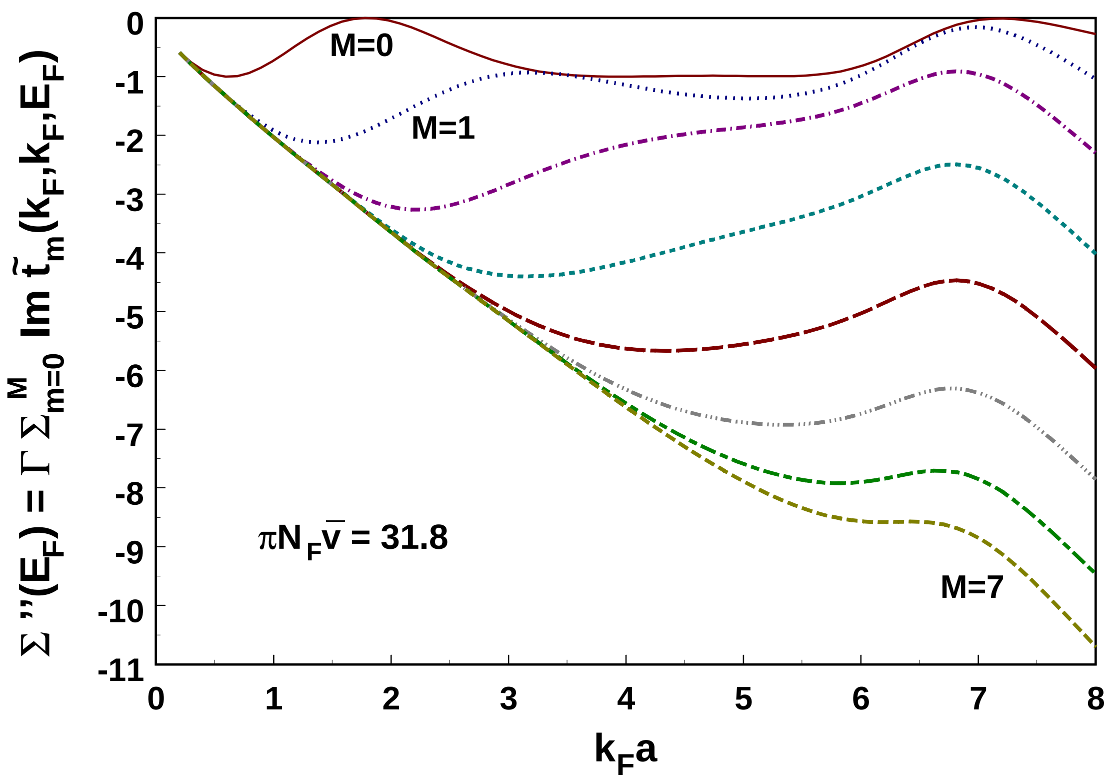

Area of the scatterer, where $N(r) \ll N(\infty)$ has been rescaled.

Period of oscillations is independent of parameters describing the scattering centers!

Amplitudes of oscillations depend on the range (vanishing logarithmically for $a \longrightarrow 0$), as well as on the strength of the scattering potential.

# Results - Selfenergy / Imaginary part

**Strong potential leading to resonant scattering in the $s$- and $p$- wave channels.**



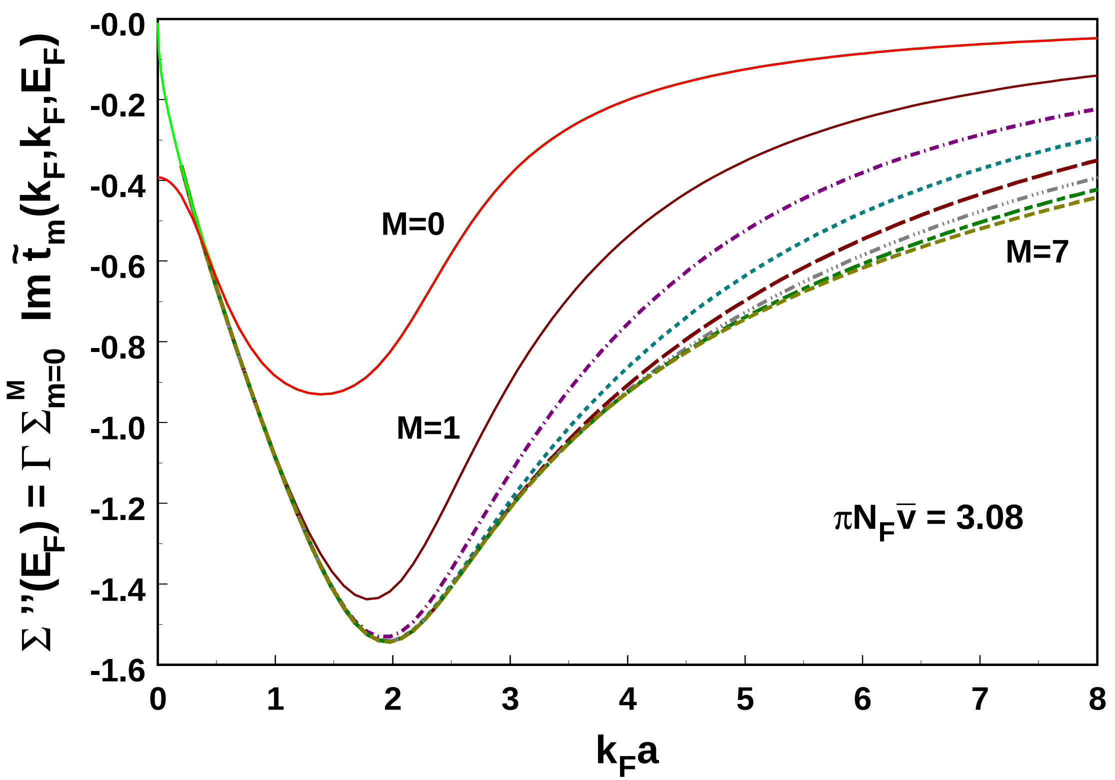

**The fully converged self-energy shows no signature of resonance scattering!**

**$\Sigma''$ increases substantially with the range. The average potential is kept constant.**

**The behavior at very large $a$ could be a numerical arte-fact.**

# Results - Selfenergy / Imaginary part

**A weaker potential with no resonant scattering.**
**The Born series still diverges, though.**




**Again $|\Sigma''|$ increases substantially with increasing range, this time to a maximum around $k_F a \approx 2$, before decreasing again.**

**The absolute values are much smaller.**

**$\Sigma''(\omega)$ near $E_F$ for (unconventional) superconductors ???**

# Summary - NFE Systems

We have shown what needs to be done to treat scattering off arbitrarily high potentials of (almost) arbitrary shape correctly and have given results for the LDOS near the defect and the selfenergy in the normal state assuming NFE.

The dependence of the selfenergy on the hight and the range of the potential is of some interest when discussing an effective scattering strength, but can hardly be checked experimentally (STM?). The easily accessible frequency dependence is very smooth in the normal state for any potential.

This changes when there is a gap in the DOS (midgap states in $d$-wave superconductors). Numerical calculations for this case have proved difficult, but will be completed soon.

# *Thanks to Coworkers*

**Dr. Carsten Rieck**

**Simon Scheffler**

**Tim Wehling (Graphene)**