Effects of disorder with finite range on the properties of d – wave superconductors

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Motivation

Advertisement: The study of disorder effects in superconductors will give information on the pairing state and the pairing interaction

Unfortunately, in the case of unconventional superconductors, theoretical predictions are **VERY** sensitive to details of disorder, e.g. strength and shape of scattering potentials.
Such studies might teach us more about the nature of the defects, as well as the correct way to describe the effects of disorder, than the superconducting state! Using approximations popular in the theory of superconductivity and taking the normal state limit can lead to unacceptable results.
Defects affect many properties, notably low temperature, low frequency transport properties.

T-Matrix (single impurity / alloy model)

$$\hat T(\boldsymbol{k},\boldsymbol{k'};\omega) = V(\boldsymbol{k}-\boldsymbol{k'})\hat\sigma_3 + \int \frac{d^2p}{(2\pi)^2} V(\boldsymbol{k}-\boldsymbol{p})\,\hat\sigma_3\,\hat G^0(\boldsymbol{p},\omega)\,\hat T(\boldsymbol{p},\boldsymbol{k'};\omega)$$ exact !

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

$$V(\boldsymbol{r}) = \sum_{i=1}^{N} v(\boldsymbol{r}-\boldsymbol{R}_i) \qquad N \gg 1 \text{ alloy model}$$

Average with respect to $\vec R_i$
Non-crossing approximation

$$\hat t(\boldsymbol{k},\boldsymbol{k'};\omega) = v(\boldsymbol{k}-\boldsymbol{k'})\hat\sigma_3 + \int \frac{d^2p}{(2\pi)^2} v(\boldsymbol{k}-\boldsymbol{p})\,\hat\sigma_3\,\hat G(\boldsymbol{p},\omega)\,\hat t(\boldsymbol{p},\boldsymbol{k'};\omega)$$

$\hat t$ is the T-Matrix for a single defect.

$$\hat G(\boldsymbol{k},\omega) = \left[\omega\hat\sigma_0 - \varepsilon(\boldsymbol{k})\hat\sigma_3 - \Delta(\boldsymbol{k})\hat\sigma_1 - \hat\Sigma(\boldsymbol{k},\omega)\right]^{-1} = G_0\,\hat\sigma_0 + G_3\,\hat\sigma_3 + G_1\,\hat\sigma_1$$

with $\hat\Sigma(\boldsymbol{k},\omega) = n_{\mathrm{imp}}\,\hat t(\boldsymbol{k},\boldsymbol{k};\omega)$

In this case, the DOS $N(\boldsymbol{r},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\left[\hat G(\boldsymbol{r},\boldsymbol{r};\omega)\right]_{11}$ is spatially constant.

T-Matrix (weak / strong scatterers)

weak scatterers, Born approximation

$$\hat T(\boldsymbol{k},\boldsymbol{k};\omega) = \int \frac{d^2p}{(2\pi)^2} V(\boldsymbol{k}-\boldsymbol{p})\,\hat\sigma_3\,\hat G^0(\boldsymbol{p},\omega)\,V(\boldsymbol{p}-\boldsymbol{k})$$

In many cases $V(\boldsymbol{k}-\boldsymbol{p})$ does not need to be specified. A few integrals involving V are parametrized. If necessary, assumptions with respect to $|V(\boldsymbol{k}-\boldsymbol{p})|^2$ are made.
Re T is irrelevant, can be absorbed in the chemical potential.
Im T involves only Im G.

strong scatterers

A detailed model for $V(\boldsymbol{k}-\boldsymbol{p})$ is required to define the kernel of the integral equation. Since T is complex, both Im $\hat G^0$ and Re $\hat G^0$ are required.

T-Matrix (point-like scatterers)

$$V(\boldsymbol{k}-\boldsymbol{p}) = V \;\Rightarrow \hat T(\omega) = \left[\left(\frac{1}{V} - \int \frac{d^2p}{(2\pi)^2} G_3(\boldsymbol{p},\omega)\right)\hat\sigma_3 - \int \frac{d^2p}{(2\pi)^2} G_0(\boldsymbol{p},\omega)\,\hat\sigma_0\right]^{-1}$$

Unconventional superconductors : Pole close to the real axis for small ω when the coefficient of $\hat\sigma_3$ vanishes. $\Rightarrow$ "resonant scattering", "midgap states"

Re $\int \frac{d^2p}{(2\pi)^2} G_3(\boldsymbol{p},\omega) = \mathrm{Re}\,\hat G_3(\boldsymbol{r}=\boldsymbol{0},\omega)$ does not exist !

Possible ways out:

- neglect the divergent contribution $G_3(\boldsymbol{r}=\boldsymbol{0},\omega)$ (invoke particle-hole symmetry). Then consider the unitary limit $V \to \infty$.
- consider only a single band of finite width
- Consider finite range scatterers, including the dependence of V on $|k|$. This way the physical origin of resonant scattering - matching of wave-length to size of scattering center - would be recovered.

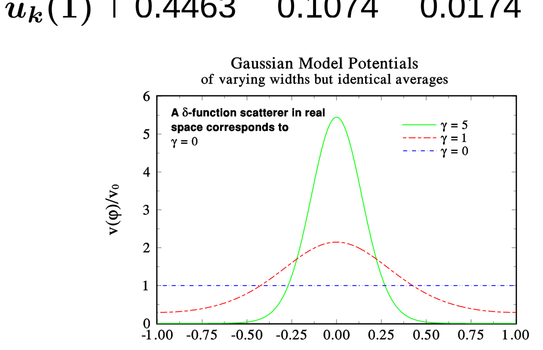
Model

Defects are described by a concentration n_{imp} and some momentum dependent model scattering potential $v(\boldsymbol{k},\boldsymbol{k'})$. In order to generalize and compare with our previous work on the conductivity we assume a circular Fermi surface and an infinitely wide band. Then the potential v is an even function of the angle φ between k_F and k'_F, which can be expanded as

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

For a Gaussian $v(\varphi) = v_0\,\frac{1}{I_0(\gamma)}\,e^{\gamma\cos\varphi}$ one has $u_k(\gamma) = I_k(\gamma)/I_0(\gamma)$

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	$< 10^{-4}$



We can also study the effect of scattering in individual ℓ–channels, by keeping only some of the coefficients u_k. These could be varied at will and, in particular, could be taken to be negative.

T-matrix (Fermi surface restricted approximation)

There are important consequences of the dependence of V on k, even if we put $|k| = k_F$. Then the equation for $\hat T = \sum_{i=1}^{n} t^i\hat\sigma_i$ reduces to

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

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

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

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

$\boldsymbol{g^0(\psi;\omega)}$ and $\boldsymbol{g^1(\psi;\omega)}$ are the energy integrated normal and anomalous retarded Green functions

$$g^0(\psi,\omega_+) = -\frac{\omega - \Sigma_0(\psi,\omega_+)}{\sqrt{[\Delta(\psi)+\Sigma_1(\psi,\omega_+)]^2 - [\omega - \Sigma_0(\psi,\omega_+)]^2}}$$

$$g^1(\psi,\omega_+) = -\frac{\Delta(\psi) + \Sigma_1(\psi,\omega_+)}{\sqrt{[\Delta(\psi)+\Sigma_1(\psi,\omega_+)]^2 - [\omega - \Sigma_0(\psi,\omega_+)]^2}}$$

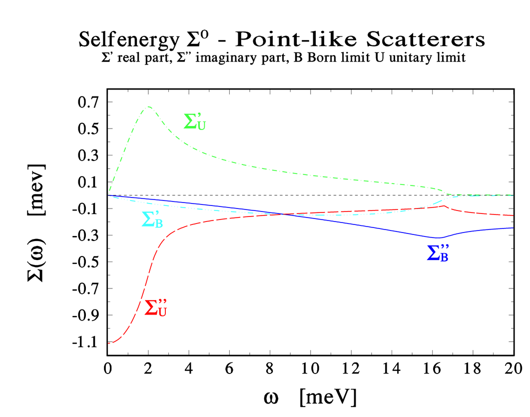
Since particle-hole symmetry is assumed, $\boldsymbol{g^0}$ and $\boldsymbol{g^1}$ are independent of $\boldsymbol{t^3(\psi,\psi)}$ and $\boldsymbol{g^3}$ vanishes. All four components $\boldsymbol{t^\ell(\varphi,\phi)}$ are required for the calculation of $\boldsymbol{\Sigma_{0,1}}$.

Selfenergy Σ^0

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

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

For point-like scatterers $\Sigma^1 = 0$ and Σ^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: $\Sigma''_B \ll \Sigma''_U$ for $\omega \to 0$.
For elevated frequencies one finds $\Sigma''_U \leq \Sigma''_B$
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)

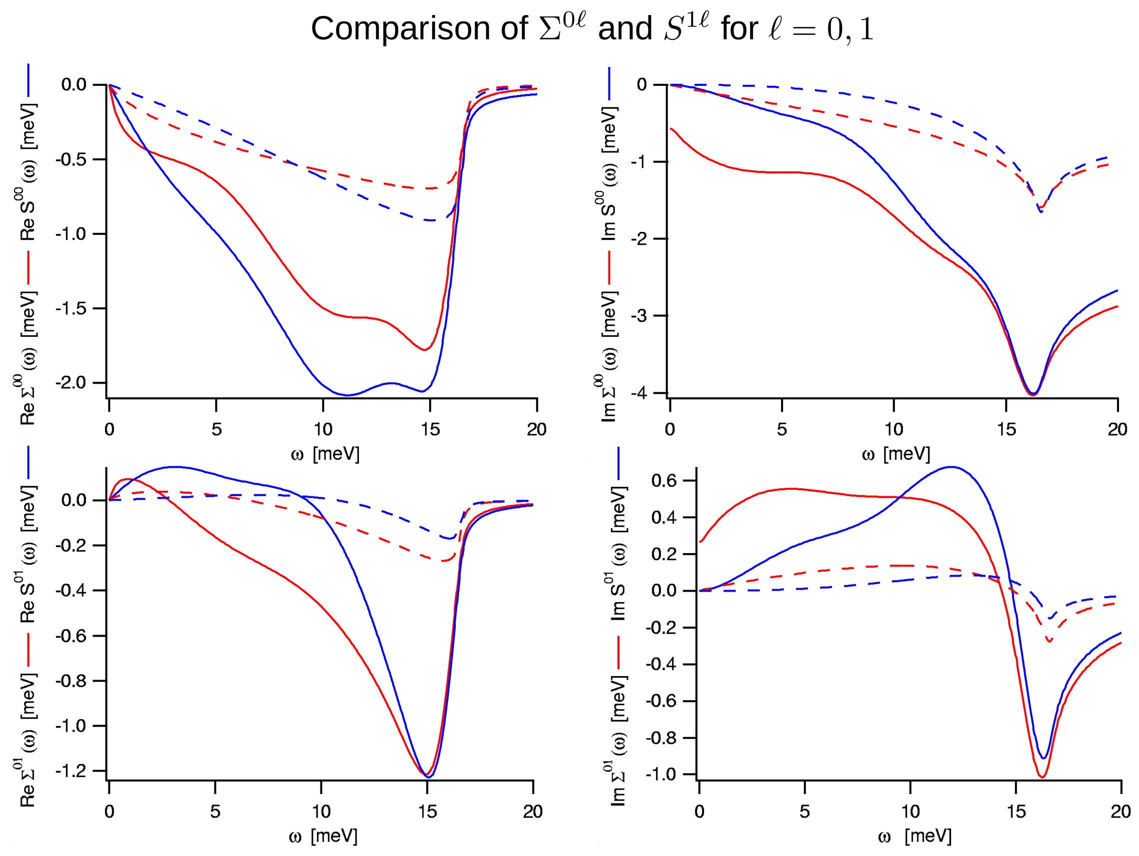
For $\omega \to \infty$, Σ''_B and Σ''_U tend to $\Gamma_{\mathrm N}^{\mathrm{el}}$, chosen to be 0.2 meV in these calculations.

Selfenergies Σ^0 and Σ^1 for Gaussian potential, $\gamma = 5$

$$\Sigma^0(\omega,\varphi) = \sum_{\ell=-\infty}^{\infty} \Sigma^{0\ell}(\omega)\,\cos[4\ell\varphi] \qquad ; \qquad \Delta(\varphi) = \Delta_0\cos[2\varphi]$$

$$\Sigma^1(\omega,\varphi) = \sum_{\ell=-\infty}^{\infty} \Sigma^{1\ell}(\omega)\,\cos[(4\ell-2)\varphi] = \frac{\Delta(\varphi)}{\omega}\sum_{\ell=-\infty}^{\infty} S^{1\ell}(\omega)\,\cos[4\ell\varphi]$$

Comparison of $\Sigma^{0\ell}$ and $S^{1\ell}$ for $\ell = 0, 1$



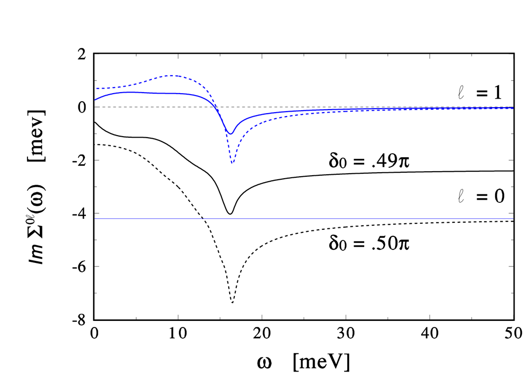
solid : $\delta_0 = 0.49\pi$, $c = 0.03$, near unitary limit dashed : $\delta_0 = 0.10\pi$, $c = 3.1$, near Born limit

The fact that $Im\,\Sigma^{00}(\omega \gg \Delta_{\max})$ near the Born limit is much larger than the corresponding value for point-like scatterers is due to the ambiguity in comparing $v = const$ and $v(\varphi)$:
$\langle v^2(\varphi)\rangle = \langle v(\varphi)\rangle^2\,I_0(2\gamma)/I_0^2(\gamma) = 3.8\,\langle v(\varphi)\rangle^2$ for $\gamma = 5$.
Note the large contribution to quasiparticle scattering at frequencies near the OP maximum!

Selfenergy Σ^0 for Gaussian potential, limiting behavior

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

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



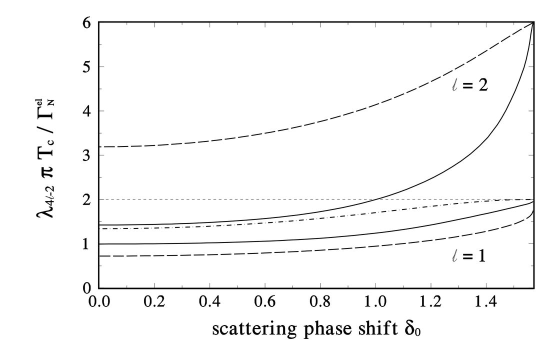
Unitary limit: $\Sigma^{00}(\delta_0 = 0.5\pi) = -i\,\Gamma_{\mathrm N}^{\mathrm{el}}\,(1+2M)$
The limiting value in the Figure is 4.2 meV since we have chosen $M = 10$.
There is a problem here with the Fermi surface restricted approach!.
For $\delta_0 = 0.49\pi$, the contribution from terms $m > 7$ 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.

T_c-reduction (one component OP)

$$\Delta(\varphi) \propto \cos(4\ell-2)\varphi \quad \Longrightarrow \quad \ln\frac{T_c}{T_{c0}} = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{\lambda_{4\ell-2}}{2}\right)$$

with pair breaking parameters $\lambda_{4\ell-2} = \frac{\Gamma_{\mathrm N}^{\mathrm{el}}}{\pi T_c}\,\frac{1}{2}\sum_{m=-\infty}^{\infty}\frac{(u_m - u_{m+4\ell-2})^2}{(\cos^2\delta_0 + u_m^2\sin^2\delta_0)(1+u_{m+4\ell-2}^2\tan^2\delta_0)}$



Pair breaking parameters λ_2 and λ_6 for Gaussian potentials with widths $\gamma = 1$ (solid lines) and $\gamma = 5$ (dashed lines) as function of the s–wave scattering phase shift $\delta_0 = \tan^{-1}(\pi N_F v_0)$. The dot-dashed line is obtained for $\gamma = 5$ when only $s-$, $p-$, and $d-$wave scattering are taken into account. When $\gamma = 1$, the difference between this approximation and the full expansion is hardly visible.

T_c-reduction (pair breaking - Born limit)

Pair breaking parameter, Born limit $\delta_0 \to 0$

$$\lambda^{\mathrm{Born}}_{4\ell-2} = \frac{\Gamma_{\mathrm N}^{\mathrm{el}}}{\pi T_c}\,\frac{1}{2}\sum_{m=-\infty}^{\infty}(u_m - u_{m+4\ell-2})^2$$

$$= \frac{n_{imp}}{\pi T_c}\,\pi N_F \int_0^{2\pi}\frac{d\varphi}{2\pi}\,v^2(\varphi)\,\{\,1 - \cos([4\ell-2]\,\varphi)\,\}$$

$$= \frac{\Gamma_{\mathrm N}^{\mathrm{el}}}{\pi T_c}\,\frac{1}{I_0^2(\gamma)}\,[\,I_0(2\gamma) - I_{4\ell-2}(2\gamma)\,] \qquad \text{for Gaussian potential}$$

If only the first three terms are taken into account one finds for $\ell = 1$

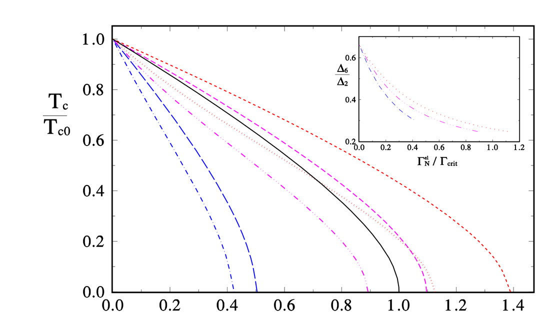
$$\lambda_2^{\mathrm{Born}} = \frac{\Gamma_{\mathrm N}^{\mathrm{el}}}{\pi T_c}\,\left[(1-u_2)^2 + u_2^2 + u_1^2\right] = \frac{\Gamma_{\mathrm N}^{\mathrm{el}}}{\pi T_c}\,\frac{1}{I_0^2(\gamma)}\,\left[\,(I_0(\gamma) - I_2(\gamma))^2 + I_2^2(\gamma) + I_1^2(\gamma)\,\right]$$

which could be very different for large γ. For extended defects, the Born approximation does not result from the T-Matrix by simply omitting the denominators.

T_c-reduction (two component OP)

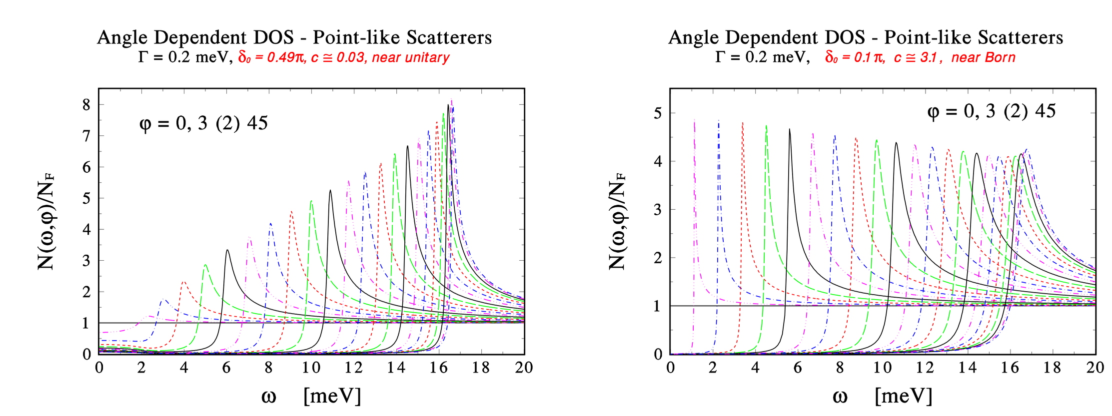
$\boldsymbol{\Delta(\varphi) \propto c_2\cos 2\varphi + c_6\cos 6\varphi}$ (popular ansatz to explain U-shape in ARPES)

$$\ln\frac{\omega_D}{2\pi T_c} = \frac{1}{2}\left[\frac{1}{\lambda_+} + \frac{1}{\lambda_-} + \psi\left(\frac{1}{2}+\frac{\lambda_2}{2}\right) + \psi\left(\frac{1}{2}+\frac{\lambda_6}{2}\right)\right] \pm \frac{1}{2}\left[\left(\frac{1}{\lambda_+} - \frac{1}{\lambda_-}\right)^2 + \left(\psi\left(\frac{1}{2}+\frac{\lambda_2}{2}\right) - \psi\left(\frac{1}{2}+\frac{\lambda_6}{2}\right)\right)^2 \psi\left(\frac{1}{2}+\frac{\lambda_2}{2}\right) - \psi\left(\frac{1}{2}+\frac{\lambda_6}{2}\right)\Bigg)\left(\frac{1}{\lambda_+} + \frac{1}{\lambda_-}\right)\frac{\Lambda_{22}-\Lambda_{66}}{\Lambda_{22}+\Lambda_{66}}\right]^{\frac{1}{2}}$$

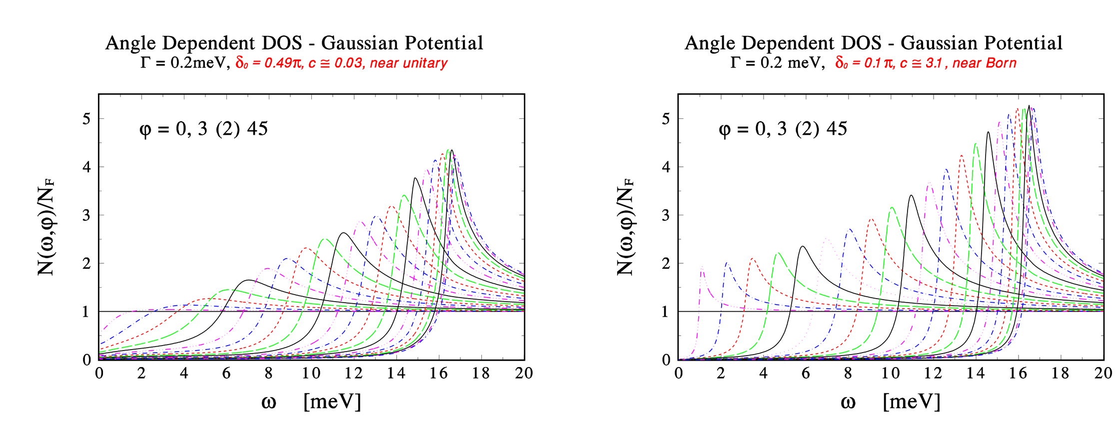


Critical temperature T_c for Gaussian potential with width $\gamma = 5$ for three different phase shift $\delta_0 = 0.05\pi, 0.3\pi, 0.5\pi$.
full line : Abrikosov-Gorkov
dashed lines : single component OP
dot-(dash) lines : two component OP
Inset depends on details of the pairing interaction; It can happen that $\Delta_6/\Delta 2$ remains constant.

Angle Dependent DOS – Spectralfunction



These curves reflect the frequency dependence of Σ''_U and Σ''_B



$N(\omega,\varphi)$ at $\omega \approx 0$ and $\omega \approx \Delta_{\max} = 16.6$ meV depends sensitively on strength and shape of the scattering potential!

Summary

- T-Matrix
  - single impurity / alloy model: almost identical calculations
  - weak / strong scatterers; point like / extended scatterers: The assumption of point like scatterers causes no problems, when the scattering is weak. For resonant scattering, Re $\hat G$ and the dependence of V on $|k|$ needs to be taken into account
- Results for a Fermi surface restricted approximation
  - T_c-reduction: is mitigated by d-wave scattering only in the Born limit. $T_c(\Gamma_{\mathrm N}^{\mathrm{el}})$ qualitativ similar to AG , unless the OP has several components.
  - Density of States: The appearance of resonances depends sensitively on the shape of the scattering potential. Most likely, the finite range of the scattering potential will reduce $N(\omega = 0)$.