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# Memorandum

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## MUSRFIT plug-in for the calculation of the temperature dependence of $1/\lambda^2$ for various gap symmetries

This memo is intended to give a short summary of the background on which the GapIntegrals plug-in for musrfit [1] has been developed. The aim of this implementation is the efficient calculation of integrals of the form

$$I(T) = 1 + \frac{1}{\pi}\int_0^{2\pi}\int_{\Delta(\varphi,T)}^{\infty}\left(\frac{\partial f}{\partial E}\right)\frac{E}{\sqrt{E^2-\Delta^2(\varphi,T)}}\mathrm{d}E\mathrm{d}\varphi\,, \tag{1}$$

where $f = (1+\exp(E/k_\mathrm{B}T))^{-1}$, like they appear e.g. in the theoretical temperature dependence of $1/\lambda^2$ [4]. For gap symmetries which involve not only a $E$- and $\varphi$-dependence but also a $\theta$-dependence, see the special section towards the end of the memo. In order not to do too many unnecessary function calls during the final numerical evaluation we simplify the integral (1) as far as possible analytically. The derivative of $f$ is given by

$$\frac{\partial f}{\partial E} = -\frac{1}{k_\mathrm{B}T}\frac{\exp(E/k_\mathrm{B}T)}{(1+\exp(E/k_\mathrm{B}T))^2} = -\frac{1}{4k_\mathrm{B}T}\frac{1}{\cosh^2(E/2k_\mathrm{B}T)}. \tag{2}$$

Using (2) and doing the substitution $E'^2 = E^2 - \Delta^2(\varphi,T)$, equation (1) can be written as

$$\begin{aligned} I(T) &= 1 - \frac{1}{4\pi k_\mathrm{B}T}\int_0^{2\pi}\int_{\Delta(\varphi,T)}^{\infty}\frac{1}{\cosh^2(E/2k_\mathrm{B}T)}\frac{E}{\sqrt{E^2-\Delta^2(\varphi,T)}}\mathrm{d}E\mathrm{d}\varphi \\ &= 1 - \frac{1}{4\pi k_\mathrm{B}T}\int_0^{2\pi}\int_0^{\infty}\frac{1}{\cosh^2\left(\sqrt{E'^2+\Delta^2(\varphi,T)}/2k_\mathrm{B}T\right)}\mathrm{d}E'\mathrm{d}\varphi\,. \end{aligned} \tag{3}$$

Since a numerical integration should be performed and the function to be integrated is exponentially approaching zero for $E' \to \infty$ the infinite $E'$ integration limit can be replaced by a cutoff energy $E_\mathrm{c}$ which has to be chosen big enough:

$$I(T) \simeq \tilde{I}(T) \equiv 1 - \frac{1}{4\pi k_\mathrm{B}T}\int_0^{2\pi}\int_0^{E_\mathrm{c}}\frac{1}{\cosh^2\left(\sqrt{E'^2+\Delta^2(\varphi,T)}/2k_\mathrm{B}T\right)}\mathrm{d}E'\mathrm{d}\varphi\,. \tag{4}$$

In the case that $\Delta^2(\varphi,T)$ is periodic in $\varphi$ with a period of $\pi/2$ (valid for all gap symmetries implemented at the moment), it is enough to limit the $\varphi$-integration to one period and to multiply the result by 4:

$$\tilde{I}(T) = 1 - \frac{1}{\pi k_\mathrm{B}T}\int_0^{\pi/2}\int_0^{E_\mathrm{c}}\frac{1}{\cosh^2\left(\sqrt{E'^2+\Delta^2(\varphi,T)}/2k_\mathrm{B}T\right)}\mathrm{d}E'\mathrm{d}\varphi\,. \tag{5}$$

For the numerical integration we use algorithms of the Cuba library [2] which require to have a Riemann integral over the unit square. Therefore, we have to scale the integrand by the upper limits of the integrations. Note that $E_\mathrm{c}$ and $\pi/2$ (or in general the upper limit of the $\varphi$ integration) are now treated as dimensionless scaling factors.

$$\tilde{I}(T) = 1 - \frac{E_\mathrm{c}}{2k_\mathrm{B}T}\int_0^{1_\varphi}\int_0^{1_E}\frac{1}{\cosh^2\left(\sqrt{(E_\mathrm{c}E)^2+\Delta^2\left(\frac{\pi}{2}\varphi,T\right)}/2k_\mathrm{B}T\right)}\mathrm{d}E\mathrm{d}\varphi \tag{6}$$

## Implemented gap functions and function calls from MUSRFIT

Currently the calculation of $\tilde{I}(T)$ is implemented for various gap functions. The temperature dependence of the gap functions is either given by Eq.(7) [3], or by Eq.(8) [4].

**A few words of warning:** The temperature dependence of the gap function is typically derived from within the BCS framework, and strongly links $T_c$ and $\Delta_0$ (e.g. $\Delta_0 = 1.76\, k_B T_c$ for an s-wave superconductor). In a self-consistent description this would mean that $\Delta_0$ of $\Delta(\varphi)$ is locked to $T_c$ as well. In the implementation provided, this limitation is lifted, and therefore the *user* should judge and question the result if the ratio $\Delta_0/(k_B T_c)$ is strongly deviating from BCS values!

$$\Delta(\varphi, T) \simeq \Delta(\varphi)\, \tanh\left[c_0 \sqrt{a_G \left(\frac{T_c}{T} - 1\right)}\right] \tag{7}$$

with $\Delta(\varphi)$ as given below, and $c_0$ and $a_G$ depends on the pairing state:

***s*-wave:** $a_G = 1$ with $c_0 = \frac{\pi k_B T_c}{\Delta_0} = \pi/1.76 = 1.785$

***d*-wave:** $a_G = 4/3$ with $c_0 = \frac{\pi k_B T_c}{\Delta_0} = \pi/2.14 = 1.468$

$$\Delta(\varphi, T) \simeq \Delta(\varphi) \tanh\left[1.82 \left(1.018 \left(\frac{T_c}{T} - 1\right)\right)^{0.51}\right]. \tag{8}$$

The GapIntegrals plug-in calculates $\tilde{I}(T)$ for the following $\Delta(\varphi)$:

**s-wave gap:**

$$\Delta(\varphi) = \Delta_0 \tag{9}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapSWave 1 2 [3 4]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

**d-wave gap [5]:**

$$\Delta(\varphi) = \Delta_0 \cos(2\varphi) \tag{10}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapDWave 1 2 [3 4]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

**non-monotonic *d*-wave gap [6]:**

$$\Delta(\varphi) = \Delta_0 \left[a \cos(2\varphi) + (1 - a) \cos(6\varphi)\right] \tag{11}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapNonMonDWave1 1 2 3 [4 5]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), $a$ (1), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

**non-monotonic *d*-wave gap [7]:**

$$\Delta(\varphi) = \Delta_0 \left[\frac{2}{3}\sqrt{\frac{a}{3}} \cos(2\varphi) \,/\, \left(1 + a \cos^2(2\varphi)\right)^{\frac{3}{2}}\right],\ a > 1/2 \tag{12}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapNonMonDWave2 1 2 3 [4 5]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), $a$ (1), $a$ (1), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

**anisotropic *s*-wave gap [8]:**

$$\Delta(\varphi) = \Delta_0 \left[1 + a\cos(4\varphi)\right] \text{ , } 0 \leqslant a \leqslant 1 \tag{13}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapAnSWave 1 2 3 [4 5]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), $a$ (1), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

***p*-wave (point) [9]:**

$$\Delta(\theta, T) = \Delta(T)\sin(\theta) \tag{14}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapPointPWave 1 2 [3 4]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

***p*-wave (line) [10]:**

$$\Delta(\theta, T) = \Delta(T)\cos(\theta) \tag{15}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapLinePWave 1 2 [3 4]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

It is also possible to calculate a power law temperature dependence (in the two fluid approximation $n = 4$) and the dirty $s$-wave expression. Obviously for this no integration is needed.

**Power law return function:**

$$\frac{\lambda(0)^2}{\lambda(T)^2} = 1 - \left(\frac{T}{T_c}\right)^n \tag{16}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapPowerLaw 1 2`

Parameters: $T_c$ (K), $n$ (1)

**dirty *s*-wave [11]:**

$$\frac{\lambda(0)^2}{\lambda(T)^2} = \frac{\Delta(T)}{\Delta_0}\tanh\left[\frac{\Delta(T)}{2k_B T}\right] \tag{17}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapDirtySWave 1 2 [3 4]`

Parameters: $T_c$ (K), $\Delta_0$ (meV), [$c_0$ (1), $a_G$ (1)]. If $c_0$ and $a_G$ are provided, the temperature dependence according to Eq.(7) will be used, otherwise Eq.(8) will be utilized.

Currently there are two gap functions to be found in the code which are *not* documented here: `TGapCosSqDWave` and `TGapSinSqDWave`. For details for these gap functions (superfluid density along the $a/b$-axis within the semi-classical model assuming a cylindrical Fermi surface and a mixed $d_{x^2-y^2} + s$ symmetry of the superconducting order parameter (effectively: $d_{x^2-y^2}$ with shifted nodes and $a$-$b$-anisotropy)) see the source code.

## Gap Integrals for $\theta$-, and $(\theta, \varphi)$-dependent Gaps

First some general formulae as found in Ref. [3]. It assumes an anisotropic response which can be classified in 3 directions ($a$, $b$, and $c$).
For the case of a 2D Fermi surface (cylindrical symmetry):

$$n_{\substack{aa\\bb}}(T) = 1 - \frac{1}{2\pi k_B T}\int_0^{2\pi} \mathrm{d}\varphi \begin{matrix}\cos^2(\varphi)\\ \sin^2(\varphi)\end{matrix} \underbrace{\int_0^{\infty} \mathrm{d}\varepsilon \left\{\cosh\left[\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T}\right]\right\}^{-2}}_{=G(\Delta(\varphi),T)} \tag{18}$$

For the case of a 3D Fermi surface:

$$n_{\substack{aa\\bb}}(T) = 1 - \frac{3}{4\pi k_{\mathrm{B}}T}\int_0^1 \mathrm{d}z\,(1-z^2)\int_0^{2\pi}\mathrm{d}\varphi\begin{matrix}\cos^2(\varphi)\\ \sin^2(\varphi)\end{matrix}\cdot G(\Delta(z,\varphi),T) \tag{19}$$

$$n_{cc}(T) = 1 - \frac{3}{2\pi k_{\mathrm{B}}T}\int_0^1 \mathrm{d}z\,z^2\int_0^{2\pi}\mathrm{d}\varphi\begin{matrix}\cos^2(\varphi)\\ \sin^2(\varphi)\end{matrix}\cdot G(\Delta(z,\varphi),T) \tag{20}$$

The "powder averaged" superfluid density is then defined as

$$n_{\mathrm{S}} = \frac{1}{3}\cdot[\sqrt{n_{aa}n_{bb}} + \sqrt{n_{aa}n_{cc}} + \sqrt{n_{bb}n_{cc}}] \tag{21}$$

**Isotropic s-Wave Gap**

For the 2D/3D case this means that $\Delta$ is just a constant.
For the 2D case it follows

$$n_{\substack{aa\\bb}}(T) = 1 - \frac{1}{2k_{\mathrm{B}}T}\cdot G(\Delta,T) = n_{\mathrm{S}}(T). \tag{22}$$

This is the same as Eq.(3), assuming a $\Delta \neq f(\varphi)$.

The 3D case for $\Delta \neq f(\theta,\varphi)$:
The variable transformation $z = \cos(\theta)$ leads to $\mathrm{d}z = -\sin(\theta)\,\mathrm{d}\theta$, $z = 0 \to \theta = \pi/2$, $z = 1 \to \theta = 0$, and hence to

$$\begin{aligned}
n_{\substack{aa\\bb}}(T) &= 1 - \frac{3}{4\pi k_{\mathrm{B}}T}\underbrace{\int_0^{\pi/2}\mathrm{d}\theta\,\sin^3(\theta)}_{=2/3}\underbrace{\int_0^{2\pi}\mathrm{d}\varphi\begin{matrix}\cos^2(\varphi)\\ \sin^2(\varphi)\end{matrix}}_{=\pi}\cdot G(\Delta,T)\\
&= 1 - \frac{1}{2k_{\mathrm{B}}T}\cdot G(\Delta,T).\\
n_{cc}(T) &= 1 - \frac{3}{2\pi k_{\mathrm{B}}T}\underbrace{\int_0^{\pi/2}\mathrm{d}\theta\,\cos^2(\theta)\sin(\theta)}_{=1/3}\underbrace{\int_0^{2\pi}\mathrm{d}\varphi\begin{matrix}\cos^2(\varphi)\\ \sin^2(\varphi)\end{matrix}}_{=\pi}\cdot G(\Delta,T)\\
&= 1 - \frac{1}{2k_{\mathrm{B}}T}\cdot G(\Delta,T).
\end{aligned}$$

And hence

$$n_{\mathrm{S}}(T) = 1 - \frac{1}{2k_{\mathrm{B}}T}\cdot G(\Delta,T).$$

## License



# References

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