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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 φ-dependence but also a θ-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_{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 φ with a period of $\pi/2$ (valid for all gap symmetries implemented at the moment), it is enough to limit the φ-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_{c} and $\pi/2$ (or in general the upper limit of the φ 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 Δ_0 (e.g. $\Delta_0 = 1.76\, k_\mathrm{B} T_c$ for an s-wave superconductor). In a self-consistent description this would mean that Δ_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 $\Delta_0/(k_\mathrm{B} T_c)$ is strongly deviating from BCS values!

$$\Delta(\varphi, T) \simeq \Delta(\varphi)\, \tanh\left[c_0 \sqrt{a_\mathrm{G}\left(\frac{T_\mathrm{c}}{T} - 1\right)}\right] \tag{7}$$

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

***s*-wave:** $a_\mathrm{G} = 1$ with $c_0 = \dfrac{\pi k_\mathrm{B} T_\mathrm{c}}{\Delta_0} = \pi/1.76 = 1.785$

***d*-wave:** $a_\mathrm{G} = 4/3$ with $c_0 = \dfrac{\pi k_\mathrm{B} T_\mathrm{c}}{\Delta_0} = \pi/2.14 = 1.468$

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

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), Δ_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), Δ_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), Δ_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]:

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

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

Parameters: T_c (K), Δ_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]:

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

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

Parameters: T_c (K), Δ_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), Δ_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), Δ_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:

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

MUSRFIT theory line: `userFcn libGapIntegrals TGapPowerLaw 1 2`

Parameters: T_c (K), n (1)

dirty s-wave [11]:

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

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

Parameters: T_c (K), Δ_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 θ-, and (θ, φ)-dependent Gaps

For the most general case for which the gap-symmetry is (E, φ, θ)-dependent, the integral to be calculate takes the form

$$I = 1 + \frac{1}{2\pi}\int_0^\pi \sin(\theta)\,\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \int_{\Delta(\varphi,\theta,T)}^\infty \mathrm{d}E \left\{\left(\frac{\partial f}{\partial E}\right) \frac{E}{\sqrt{E^2 - \Delta^2(\varphi,\theta,T)}}\right\} \tag{18}$$

Gap Integrals for θ-dpendent Gaps

In case the gap-symmetry is only depending on (E,θ) the φ-integral can be carried out and Eq.(18) simplifies to

$$I(T) = 1 + \int_0^\pi \sin(\theta)\,\mathrm{d}\theta \int_{\Delta(\varphi,\theta,T)}^\infty \mathrm{d}E \left\{ \left(\frac{\partial f}{\partial E}\right) \frac{E}{\sqrt{E^2 - \Delta^2(\varphi,\theta,T)}} \right\} \tag{19}$$

Following the same simplification steps as for Eq.(1) we find

$$\tilde{I}(T) = 1 - \frac{\pi E_c}{4 k_\mathrm{B} T} \int_0^1 \mathrm{d}x \sin(\pi x) \int_0^1 \mathrm{d}F \, \frac{1}{\cosh^2\left(\sqrt{(E_c \cdot F)^2 + \Delta^2(\pi \cdot x, T)}/(2 k_\mathrm{B} T)\right)} \tag{20}$$

where $x = \theta/\pi$, and $F = E'/E_c$.

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References

[1] A. Suter, and B.M. Wojek, Physics Procedia **30**, 69 (2012). A. Suter, musrfit *User Manual*, http://lmu.web.psi.ch/musrfit/user/MUSR/WebHome.html

[2] T. Hahn, *Cuba – a library for multidimensional numerical integration*, Comput. Phys. Commun. **168** (2005) 78-95, http://www.feynarts.de/cuba/

[3] R. Prozorov and R.W. Giannetta, *Magnetic penetration depth in unconventional superconductors*, Supercond. Sci. Technol. **19** (2006) R41-R67, and Erratum in Supercond. Sci. Technol. **21** (2008) 082003.

[4] A. Carrington and F. Manzano, Physica C **385** (2003) 205

[5] G. Deutscher, *Andreev-Saint-James reflections: A probe of cuprate superconductors*, Rev. Mod. Phys. **77** (2005) 109-135

[6] H. Matsui *et al.*, *Direct Observation of a Nonmonotonic $d_{x^2-y^2}$-Wave Superconducting Gap in the Electron-Doped High-T_c Superconductor $Pr_{0.89}LaCe_{0.11}CuO_4$*, Phys. Rev. Lett. **95** (2005) 017003

[7] I. Eremin, E. Tsoncheva, and A.V. Chubukov, *Signature of the nonmonotonic d-wave gap in electron-doped cuprates*, Phys. Rev. B **77** (2008) 024508

[8] ??

[9] G.M. Pang, *et al.*, Phys. Rev. B **91** (2015) 220502(R), and references in there.

[10] M. Ozaki, *et al.*, Prog. Theor. Phys. **75** (1986) 442.

[11] M. Tinkham, *Introduction to Superconductivity* 2$^{\mathrm{nd}}$ ed. (Dover Publications, New York, 2004).

[12] http://www.gnu.org/licenses/old-licenses/gpl-2.0.html