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Memorandum

Date: September 19, 2009 / August 19, 2014

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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 developped. 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]. 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

At the moment the calculation of $\tilde{I}(T)$ is implemented for various gap functions all using the approximate BCS temperature dependence [3]

$$\Delta(\varphi, T) \simeq \Delta(\varphi, 0)\, \tanh\left[\frac{\pi k_\mathrm{B} T_\mathrm{c}}{\Delta_0}\sqrt{a_\mathrm{G}\left(\frac{T_\mathrm{c}}{T}-1\right)}\right] \tag{7}$$

with Δ_0 as given below, and a_G depends on the pairing state:

***s*-wave:** $a_\mathrm{G} = 1$ with $\Delta_0 = 1.76\, k_\mathrm{B} T_c$

***d*-wave:** $a_\mathrm{G} = 4/3$ with $\Delta_0 = 2.14\, k_\mathrm{B} T_c$

Eq.(7) replaces the *previously* used approximation [4]:

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

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]`
(Parameters: T_c (K), Δ_0 (meV), [a_G (1)], if a_G is not given, $a_\mathrm{G} = 1$)

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

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

MUSRFIT theory line: `userFcn libGapIntegrals TGapDWave 1 2 [3]`
(Parameters: T_c (K), Δ_0 (meV), [a_G (1)], if a_G is not given, $a_\mathrm{G} = 4/3$)

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]`
(Parameters: T_c (K), Δ_0 (meV), a (1), [a_G (1)], if a_G is not given, $a_\mathrm{G} = 4/3$)

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]`
(Parameters: T_c (K), Δ_0 (meV), a (1), a (1), [a_G (1)], if a_G is not given, $a_\mathrm{G} = 4/3$)

anisotropic *s*-wave gap [8]:

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

MUSRFIT theory line: `userFcn libGapIntegrals TGapAnSWave 1 2 3 [4]`
(Parameters: T_c (K), Δ_0 (meV), a (1), [a_G (1)], if a_G is not given, $a_\mathrm{G} = 1$)

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:

$$\frac{\lambda(0)^2}{\lambda(T)^2} = 1 - \left(\frac{T}{T_\mathrm{c}}\right)^n \tag{14}$$

MUSRFIT theory line: `userFcn libGapIntegrals TGapPowerLaw 1 2`
(Parameters: T_c (K), n (1))

dirty *s*-wave [9]:

$$\frac{\lambda(0)^2}{\lambda(T)^2} = \frac{\Delta(T)}{\Delta_0} \tanh\left[\frac{\Delta(T)}{2k_{\mathrm{B}}T}\right] \tag{15}$$

with $\Delta(T)$ given by Eq.(7).
MUSRFIT theory line: `userFcn libGapIntegrals TGapDirtySWave 1 2 [3]`
(Parameters: T_{c} (K), Δ_0 (meV), [a_{G} (1)], if a_{G} is not given, $a_{\mathrm{G}} = 1$)

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.

License

References

[1] A. Suter, MUSRFIT *User Manual*, https://wiki.intranet.psi.ch/MUSR/MusrFit

[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] M. Tinkham, *Introduction to Superconductivity* 2nd ed. (Dover Publications, New York, 2004).

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