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Memorandum

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An: To whom it may concern

cc:

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 $1/\lambda^2$ [3]. 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

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

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

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

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]

$$\Delta(\varphi, T) \simeq \Delta(\varphi) \tanh\left(1.82\left(1.018\left(\frac{T_{\mathrm{c}}}{T}-1\right)\right)^{0.51}\right). \tag{7}$$

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

s-wave gap: $\Delta(\varphi) = \Delta_0$
MUSRFIT theory line[1]: `userFcn libGapIntegrals.so TGapSWave 1 2` (Parameters: T_{c} Δ_0)

d-wave gap [4]: $\Delta(\varphi) = \Delta_0 \cos(2\varphi)$
MUSRFIT theory line: `userFcn libGapIntegrals.so TGapDWave 1 2` (Parameters: T_{c} Δ_0)

non-monotonic d-wave gap [5]: $\Delta(\varphi) = \Delta_0 \left[a \cos(2\varphi) + (1-a)\cos(6\varphi)\right]$
MUSRFIT theory line: `userFcn libGapIntegrals.so TGapNonMonDWave1 1 2 3` (Parameters: T_{c} Δ_0 a)

non-monotonic d-wave gap [6]: $\Delta(\varphi) = \Delta_0 \left[\frac{2}{3}\sqrt{\frac{a}{3}}\cos(2\varphi) \,/\, \left(1 + a\cos^2(2\varphi)\right)^{\frac{3}{2}}\right]$, $a > 1/2$
MUSRFIT theory line: `userFcn libGapIntegrals.so TGapNonMonDWave2 1 2 3` (Parameters: T_{c} Δ_0 a)

anisotropic s-wave gap [7]: $\Delta(\varphi) = \Delta_0 \left[1 + a\cos(4\varphi)\right]$, $0 \leqslant a \leqslant 1$
MUSRFIT theory line: `userFcn libGapIntegrals.so TGapAnSWave 1 2 3` (Parameters: T_{c} Δ_0 a)

It is also possible to calculate a power law temperature dependence; obviously for this no integration is needed.

Power law return function: $1 - \left(\frac{T}{T_{\mathrm{c}}}\right)^n$
MUSRFIT theory line: `userFcn libGapIntegrals.so TGapPowerLaw 1 2` (Parameters: T_{c} n)

License

The GapIntegrals library has been released under the GNU General Public License, Version 2 [8] – please make sure to comply with it.

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

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

[5] 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

[6] 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

[7]

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

[1] valid under Linux – under MS Windows the GapIntegrals library might have the extension .dll, under MacOSX .dylib

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