Numerical computation of the BCS gap function and other related functions

Erkki Thuneberg
Department of Physics, P.O.Box 3000, FI-90014 University of Oulu, Finland

R. Hänninen
Low Temperature Laboratory, Helsinki University of Technology, P.O.Box 2200, 02015 HUT, Finland
(Dated: January 14, 2025)

I. INTRODUCTION

We give formulas for efficient numerical computation of the BCS gap function and other related functions. Computer codes in different formats are available in Ref. [1].

II. SUPERCONDUCTIVITY (S-WAVE) AND ^{3}He-B

The BCS gap function $\Delta(T)$ is defined by the gap equation[2]. In the simplest case (s-wave or p-wave for pure superfluid ^{3}He-B) the equation has the form $G = 0$, where

$$G(\Delta) = \ln\frac{T}{T_c} + \pi k_B T \sum_{\epsilon_n}\left[\frac{1}{|\epsilon_n|} - \frac{1}{\sqrt{\epsilon_n^2+\Delta^2}}\right], \tag{1}$$

$\epsilon_n = 2\pi k_B T(n-\frac{1}{2})$ and $n = 0, \pm 1, ... \pm\infty$. Introducing $t = T/T_c$ and $y = \Delta/2\pi k_B T_c$, this equals

$$G(y) = \ln t + \sum_{n=1}^{\infty}\left[\frac{1}{n-\frac{1}{2}} - \frac{t}{\sqrt{t^2(n-\frac{1}{2})^2+y^2}}\right]. \tag{2}$$

In order to solve this, the sum has to be calculated exactly at least for the lowest n. However, very many terms in the sum are required at low temperatures. In order to solve the gap equation accurately and effectively at all temperatures, the following procedure can be used. For the first m terms the sum is calculated exactly. The remaining terms are approximated by an integral using the Euler-MacLaurin formula

$$\sum_{n=m_1}^{m_2-1} f(n+\frac{1}{2}) = \int_{m_1}^{m_2} ds f(s) + \frac{1}{24}[f'(m_1) - f'(m_2)] + O(f'''). \tag{3}$$

This gives

$$G(y) = \sum_{n=1}^{m}\left[\frac{1}{n-\frac{1}{2}} - \frac{t}{\sqrt{t^2(n-\frac{1}{2})^2+y^2}}\right] + \ln\frac{mt+\sqrt{m^2t^2+y^2}}{2m} - \frac{1}{24}\left[\frac{1}{m^2} - \frac{mt^3}{(m^2t^2+y^2)^{3/2}}\right] + O(\frac{1}{m^4}). \tag{4}$$

It should be noted that this expression can straightforwardly be programmed and it is nonsingular even at $t = 0$. An alternative form for (4) is obtained by summing the $(n-\frac{1}{2})^{-1}$ term exactly

$$G(y) = -\sum_{n=1}^{m}\frac{t}{\sqrt{t^2(n-\frac{1}{2})^2+y^2}} + \ln 2e^{\gamma} + \ln(mt+\sqrt{m^2t^2+y^2}) + \frac{mt^3}{24(m^2t^2+y^2)^{3/2}} + O(\frac{1}{m^4}) \tag{5}$$

where the Euler gamma $\gamma = 0.577215664$. ($G(y) = \ln(2e^{\gamma}y)$ at $t = 0$.) From (4) one can also easily calculate the derivative

$$\frac{dG}{dy}(y) = \sum_{n=1}^{m}\frac{ty}{[t^2(n-\frac{1}{2})^2+y^2]^{3/2}} + \frac{y}{\sqrt{m^2t^2+y^2}(mt+\sqrt{m^2t^2+y^2})} - \frac{mt^3y}{8(m^2t^2+y^2)^{5/2}} + O(\frac{1}{m^6}), \tag{6}$$

which is needed in applying the Newton iteration

$$y^{(n+1)} = y^{(n)} - \frac{G(y^{(n)})}{dG/dy(y^{(n)})}. \tag{7}$$

Numerical test shows that very high accuracy is achieved with moderate $m = 10$ at all temperatures.

In superfluid ^{3}He-B one often needs the following functions[3]. The temperature dependent functions Z_j are defined by

$$Z_j = \pi k_B T \Delta^{j-1} \sum_{\epsilon_n} (\epsilon_n^2 + \Delta^2)^{-j/2} \tag{8}$$

using the same principle as above these sums can be written effectively as

$$Z_3 = y^2 \left[\sum_{n=1}^{m} \frac{t}{[t^2(n-\frac{1}{2})^2 + y^2]^{3/2}} + \frac{1}{\sqrt{m^2t^2+y^2}(mt + \sqrt{m^2t^2+y^2})} - \frac{mt^3}{8(m^2t^2+y^2)^{5/2}} \right] + O(\frac{1}{m^6}), \tag{9}$$

$$Z_5 = y^4 \left[\sum_{n=1}^{m} \frac{t}{[t^2(n-\frac{1}{2})^2 + y^2]^{5/2}} + \frac{mt + 2\sqrt{m^2t^2+y^2}}{3(m^2t^2+y^2)^{3/2}(mt + \sqrt{m^2t^2+y^2})^2} - \frac{5mt^3}{24(m^2t^2+y^2)^{7/2}} \right] + O(\frac{1}{m^8}), \tag{10}$$

$$Z_7 = y^6 \left[\sum_{n=1}^{m} \frac{t}{[t^2(n-\frac{1}{2})^2 + y^2]^{7/2}} + \frac{11m^2t^2 + 9mt\sqrt{m^2t^2+y^2} + 8y^2}{15(m^2t^2+y^2)^{5/2}(mt + \sqrt{m^2t^2+y^2})^3} - \frac{7mt^3}{24(m^2t^2+y^2)^{9/2}} \right] + O(\frac{1}{m^{10}}). \tag{11}$$

The $\lambda(T)$ function is defined by

$$\lambda = \pi k_B T \sum_{\epsilon_n} \frac{\Delta}{\sqrt{\epsilon_n^2 + \Delta^2}(\sqrt{\epsilon_n^2 + \Delta^2} + \Delta)}. \tag{12}$$

Applying the same method gives

$$\begin{aligned} \lambda = & \sum_{n=1}^{m} \frac{ty}{\sqrt{t^2(n-\frac{1}{2})^2 + y^2}(y + \sqrt{t^2(n-\frac{1}{2})^2 + y^2})} + 1 - \frac{mt}{y + \sqrt{m^2t^2+y^2}} \\ & - \frac{mt^3 y(y + 2\sqrt{m^2t^2+y^2})}{24(m^2t^2+y^2)^{3/2}(y + \sqrt{m^2t^2+y^2})^2} + O(\frac{1}{m^5}). \end{aligned} \tag{13}$$

Let us apply the Euler-MacLaurin formula also to the Ginzburg-Landau theory of impure ^{3}He[4]. Here we use $t = T/T_{c0}$, $z = \hbar v_F / 4\pi k_B T_{c0} \ell = \xi_0 / 2\ell$, $\xi_0 = \hbar v_F / 2\pi k_B T_{c0}$, $\gamma = K'/K$ and get

$$\alpha = \frac{N(0)}{3} \sum_{n=1}^{m} \frac{z}{(n-\frac{1}{2})[t(n-\frac{1}{2}) + z]} + \ln(t + \frac{z}{m}) - \frac{1}{24m^2} + \frac{t^2}{24(tm+z)^2} + O(\frac{1}{m^4}) \tag{14}$$

$$a = \frac{N(0)}{3} \frac{1}{10(2\pi T_{c0})^2} \left[\sum_{n=1}^{m} \frac{t}{[t(n-\frac{1}{2}) + z]^3} + \frac{1}{2(tm+z)^2} + O(\frac{1}{m^4}) \right] \tag{15}$$

$$b = \frac{N(0)}{3} \frac{z}{6(2\pi T_{c0})^2} (\tilde{\sigma} - \tfrac{1}{2}) \left[\sum_{n=1}^{m} \frac{t}{[t(n-\frac{1}{2}) + z]^4} + \frac{1}{3(tm+z)^3} + O(\frac{1}{m^5}) \right] \tag{16}$$

$$K = \frac{N(0)}{3} \frac{\xi_0^2}{20} \left[\sum_{n=1}^{m} \frac{t}{[t(n-\frac{1}{2}) + z]^3} + \frac{1}{2(tm+z)^2} + O(\frac{1}{m^4}) \right] \tag{17}$$

$$K' = 3K + \frac{N(0)}{3} \frac{z\xi_0^2}{12} \left[\sum_{n=1}^{m} \frac{1}{(n-\frac{1}{2})[t(n-\frac{1}{2}) + z]^3} + \frac{1}{z^3} \ln(1 + \frac{z}{tm}) - \frac{1}{z^2(tm+z)} - \frac{1}{2z(tm+z)^2} + O(\frac{1}{m^5}) \right] \tag{18}$$

The energy functional[5]

$$
\begin{aligned}
F - F_n &= VN(0)\left[\Delta^2 \ln\frac{T}{T_c} + \pi k_B T \sum_{\epsilon_n} \frac{\Delta^4}{|\epsilon_n|(|\epsilon_n| + \sqrt{\epsilon_n^2+\Delta^2})^2}\right] \\
&= VN(0)\Delta^2\left[\ln t + \sum_{n=1}^{\infty} \frac{y^2}{(n-\frac{1}{2})\left[t(n-\frac{1}{2}) + \sqrt{t^2(n-\frac{1}{2})^2+y^2}\right]^2}\right] \\
&= VN(0)\Delta^2\left[\sum_{n=1}^{m} \frac{y^2}{(n-\frac{1}{2})\left[t(n-\frac{1}{2}) + \sqrt{t^2(n-\frac{1}{2})^2+y^2}\right]^2} + \frac{mt}{mt+\sqrt{m^2t^2+y^2}} - \frac{1}{2}\right. \\
&\quad \left. + \ln\frac{mt+\sqrt{m^2t^2+y^2}}{2m} - \frac{y^2(2mt+\sqrt{m^2t^2+y^2})}{24m^2\sqrt{m^2t^2+y^2}(mt+\sqrt{m^2t^2+y^2})^2} + O(\frac{1}{m^5})\right] \qquad (19)
\end{aligned}
$$

III. SUPERFLUID ^{3}He-A

For the anisotropic A phase of ^{3}He the gap equation (1) takes the form

$$G(\Delta) = \ln\frac{T}{T_c} + \pi k_B T \sum_{\epsilon_n}\left[\frac{1}{|\epsilon_n|} - \frac{3}{2}\left\langle \frac{\sin^2\theta}{\sqrt{\epsilon_n^2+\Delta^2\sin^2\theta}}\right\rangle\right], \qquad (20)$$

where the angular average is marked by $\langle f(\theta)\rangle = \int_0^1 d(\cos\theta) f(\theta)$. Now Δ is the maximum value for the energy gap. By carrying out the angular integral one obtains

$$G(y) = \ln t + \sum_{n=1}^{\infty}\left[\frac{1}{n-\frac{1}{2}} - \frac{3t}{4y^3}\left[t(n-\tfrac{1}{2})y + \left(y^2 - t^2(n-\tfrac{1}{2})^2\right)\arctan\left(\frac{y}{t(n-\frac{1}{2})}\right)\right]\right]. \qquad (21)$$

By applying the Euler-MacLaurin formula this becomes

$$
\begin{aligned}
G(y) &= \sum_{n=1}^{m}\left[\frac{1}{n-\frac{1}{2}} - \frac{3t}{4y^3}\left[t(n-\tfrac{1}{2})y + \left(y^2 - t^2(n-\tfrac{1}{2})^2\right)\arctan\left(\frac{y}{t(n-\frac{1}{2})}\right)\right]\right] - \frac{5}{6} - \frac{1}{24m^2} \\
&\quad + \frac{m^2t^2((4m^2-1)t^2+4y^2)}{16y^2(m^2t^2+y^2)} + \frac{mt((1-4m^2)t^2+12y^2)\arctan\left(\frac{y}{mt}\right)}{16y^3} + \ln\frac{\sqrt{m^2t^2+y^2}}{m}, \qquad (22)
\end{aligned}
$$

which implies that

$$
\begin{aligned}
\frac{dG(y)}{dy} &= \frac{3t}{4y^4}\sum_{n=1}^{m}\left[\frac{t(n-\frac{1}{2})y(3t^2(n-\frac{1}{2})^2+y^2)}{t^2(n-\frac{1}{2})^2+y^2} + \left(y^2 - 3t^2(n-\tfrac{1}{2})^2\right)\arctan\left(\frac{y}{t(n-\frac{1}{2})}\right)\right] \\
&\quad + \frac{1}{y} + \frac{m^2t^2}{16y^3}\left(\frac{3m^2t^4+5t^2y^2}{(m^2t^2+y^2)^2} - 12\right) + \frac{3mt}{16y^4}\left((4m^2-1)t^2 - 4y^2\right)\arctan\left(\frac{y}{mt}\right) \qquad (23)
\end{aligned}
$$

The Cross functions[6] are defined by

$$\alpha = \frac{3}{8}\left\langle \sin^2\theta\,\phi(\theta)\right\rangle \qquad (24)$$

$$\beta = \frac{3}{2}\left\langle \cos^2\theta\,\phi(\theta)\right\rangle \qquad (25)$$

$$\gamma = 3\left\langle \frac{\cos^4\theta}{\sin^2\theta}\phi(\theta)\right\rangle, \qquad (26)$$

where

$$\phi(\theta) = \pi k_B T \sum_{\epsilon_n} \frac{\Delta^2\sin^2\theta}{(\epsilon_n^2+\Delta^2\sin^2\theta)^{3/2}} \qquad (27)$$

Calculating the angular integral and using the Euler-MacLaurin formula one may find that

$$\alpha = \frac{3t}{16y^3}\sum_{n=1}^{m}\frac{t(n-\frac{1}{2})y(3t^2(n-\frac{1}{2})^2+y^2)+(y^4-2y^2t^2(n-\frac{1}{2})^2-3t^4(n-\frac{1}{2})^4)\arctan\left(\frac{y}{t(n-\frac{1}{2})}\right)}{y^2+t^2(n-\frac{1}{2})^2}$$
$$+\frac{1}{4}+\frac{m^2t^2}{64y^2}\left(\frac{3m^2t^4+5t^2y^2}{(m^2t^2+y^2)^2}-12\right)+\frac{3mt((4m^2-1)t^2-4y^2)\arctan\left(\frac{y}{mt}\right)}{64y^3} \quad (28)$$

$$\beta = \frac{3t}{4y^3}\sum_{n=1}^{m}\left[\left(3t^2(n-\tfrac{1}{2})^2+y^2\right)\arctan\left(\frac{y}{t(n-\frac{1}{2})}\right)-3t(n-\tfrac{1}{2})y\right]$$
$$+\frac{((4m^2-1)t^2+4y^2)\left(3m^2t^2y+2y^3-3mt(m^2t^2+y^2)\arctan\left(\frac{y}{mt}\right)\right)}{16y^3(m^2t^2+y^2)} \quad (29)$$

$$\gamma = 3\sum_{n=1}^{m}\left[\frac{1}{n-\frac{1}{2}}+\frac{3t}{2y^3}\left(t(n-\tfrac{1}{2})y-\left(t^2(n-\tfrac{1}{2})^2+y^2\right)\arctan\left(\frac{y}{t(n-\frac{1}{2})}\right)\right)\right]-\frac{1}{8m^2}$$
$$+\frac{3t^2}{8y^2}(1-4m^2)+\frac{3mt}{8y^3}((4m^2-1)t^2+12y^2))\arctan\left(\frac{y}{mt}\right)-4+3\ln\frac{\sqrt{y^2+m^2t^2}}{mt} \quad (30)$$

---

[1] https://users.aalto.fi/ thunebe1/theory/qc/bcsgap.html
[2] J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[3] E.V. Thuneberg, cond-mat/0005074, J. Low Temp. Phys. **122**, 657 (2001).
[4] E.V. Thuneberg, "Ginzburg-Landau Theory for Impure Superfluid ^{3}He", cond-mat/9802044
[5] J.W. Serene and D. Rainer, Phys. Rep. **101**, 221 (1983).
[6] M.C. Cross, J. Low Temp. Phys. **21**, 525 (1975).