Evaluation of the Integral $\int_0^y \frac{tanh(x)}{x}\,dx\ ; y \gg 1$ from BCS Theory in Analytic Form via Numerical Convergence Method

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Abstract

In the weak-coupling limit of superconductivity BCS theory, the energy-gap equation near the transition temperature (T_c) involves the integral $\int_0^y \frac{tanh(x)}{x}\,dx$ where $y \stackrel{\text{def}}{=} \beta_c \omega_D \gg 1$ providing k_B=Boltzmann constant and $\beta_c = (k_B\,T_c)^{-1}$ is the transition temperature parameter of this superconductor, and ω_D represents the Debye frequency of the normal-metal lattice associated with this superconductor. This integral is not simple to evaluate since its upper limit is not a constant but a variable. So far, there exists a pure analytic method to carry out this integral but complication arises. One has to deal with intuitive integration by parts and infinite series of Dirichlet Eta function. In this article we devise a new method using simple analytic and numerical techniques to carry out the integral. Based on a remarkable mathematical property that the hyperbolic tangent function may be approximated as unity for large x, we replace $tanh\,(x)$ with the new function of 2 domains separated by a critical parameter named $\tilde{x}$ between which the function takes the value of hyperbolic tangent function and unity. Suitable $\tilde{x}$ yields the correct integral. We call this "numerical convergence method". Both techniques yield the same result, *i.e.* $\int_0^y \frac{tanh(x)}{x}\,dx = Ln(1.13387\,y)\ \ ; y \gg 1.$ This result was employed further to find the ratio Cooper pair binding energy$/k_B\,T_c$.

Keywords: BCS theory, Debye frequency, Transition temperature, Cooper-pair binding energy, Numerical convergence method

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1. Introduction

Soon after Cooper (1956) discovered electron pairing, the BCS theory (Tinkham, 2004; Schrieffer, 1999; Ketterson & Song, 2010) of superconductivity followed and it was the first one that successfully explained superconductivity on microscopic scale. Due to BCS theory, the linearized BCS gap equation at the transition temperature (T_c) is, in such units that $\hbar = 1$,

$$\frac{1}{V_0\, D(\epsilon_F)} = \int_0^{\omega_D} d\xi\, \frac{\tanh\left(\frac{\beta_c}{2}\xi\right)}{\xi} \tag{1}$$

or, equivalently,

$$\frac{1}{V_0\, D(\epsilon_F)} = \int_0^{\frac{\beta_c\omega_D}{2}} dx\, \frac{\tanh(x)}{x} \tag{2}$$

where ω_D represents the Debye frequency of the metal phase, $x \equiv \frac{\beta_c}{2}\xi$ is the new variable of integration, $\beta_c \equiv \frac{1}{k_B T_c}$ stands for the temperature parameter of that superconductor calculated at the transition temperature, $D(\epsilon_F)$ is density of states of electrons at the Fermi level of the normal phase, $-V_0$ is the simplified value of matrix element $V_{\vec{k}\vec{k}'}$of the interaction between super-electrons.

Our main target is to evaluate the RHS integral of Eq.(2), which is not easy to obtain since the upper interval of integration is not a constant but a variable that depends on temperature of the superconducting material. There exists an analytic method that has been used to evaluate this integral which we are going to mention now.

This analytic method begins with performing integration by parts, yielding

$$\int_0^{\frac{\beta_c\omega_D}{2}} dx\, \frac{\tanh(x)}{x} = Ln\left(\frac{\beta_c\,\omega_D}{2}\right) \tanh\left(\frac{\beta_c\,\omega_D}{2}\right) - \int_0^{\frac{\beta_c\,\omega_D}{2}} \frac{Ln\,x}{\cosh^2 x} dx\,. \tag{3}$$

Following the original article of BCS theory, we focus on the weak-coupling limit where $\beta_c\omega_D \gg 1$ (Bardeen et al., 1957). We may, therefore, send the upper limit to infinity. We now concentrate on how to evaluate the integral $\int_0^{\infty} dx\, \frac{Ln\,x}{\cosh^2 x}$.

To do so, we first consider

$$I(s) \equiv \int_0^{\infty} \frac{x^s}{\cosh^2 x}\, dx\,. \tag{4}$$

We next observe that $I(s)$ is related to our attending integral by the expression

$$I'(0) = \int_0^\infty \frac{Ln\,x}{cosh^2\,x} dx \;. \quad (5)$$

Rewriting the hyperbolic function in exponential form gives

$$I(s) = 4\int_0^\infty \frac{x^s e^{-2x}}{(1+e^{-2x})^2}\, dx \;, \quad (6)$$

which can be written in differential form as

$$I(s) = 2\int_0^\infty x^s \frac{d}{dx}\left(\frac{1}{1+e^{-2x}}\right) dx \;. \quad (7)$$

Furthermore, the term in parenthesis can be written in geometric series form, *i.e.*

$$I(s) = 2\int_0^\infty x^s \frac{d}{dx} \sum_{k=0}^{\infty}(-e^{-2x})^k \; dx \;. \quad (8)$$

We manage to move the summation to the left and do the integral first,

$$I(s) = 4\sum_{k=1}^{\infty}(-1)^{k+1}\, k \int_0^\infty x^s e^{-2kx} \; dx \;. \quad (9)$$

The integral may now be written in the form of gamma function, we get

$$I(s) = 2^{1-s} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^s} \Gamma(s+1) \;. \quad (10)$$

Also, this infinite series may be written in the form of the Dirichlet Eta function, $\eta(s)$, so that $I(s)$ reads

$$I(s) = 2^{1-s}\, \eta(s)\, \Gamma(s+1) \;. \quad (11)$$

Then the derivative follows that

$$I'(s) = -2^{1-s}\, ln2\, \eta(s)\, \Gamma(s+1) + 2^{1-s}\, \eta'^{(s)} \Gamma(s+1) + 2^{1-s}\, \eta(s)\, \Gamma'^{(s+1)}. \quad (12)$$

Now we see that the derivative of *I* at *s=0* is

$$I'(0) = -2^{1-s}\, ln2\, \eta(0)\, \Gamma(1) + 2\,\eta'(0)\Gamma(1) + 2\,\eta(0)\,\Gamma'(1)\ . \tag{13}$$

Symbolically we obtain

$$I'(0) = Ln(\pi/4) - \gamma\ , \tag{14}$$

since we have used the values of Eta functions and its derivative at *s=0*, and also Gamma function and its derivative at *s=1* from an information source (Abramowitz & Stegun, 1972) to be

$$\eta(0) = \tfrac{1}{2},\ \Gamma(1) = 1,\ \eta'(0) = \tfrac{1}{2} Ln\left(\tfrac{\pi}{2}\right),\ \Gamma'(1) = -\gamma\ , \tag{15}$$

where $\gamma \cong \mathbf{0.577}$ is the Euler's constant.

Up to now, we are able to conclude that

$$\int_0^\infty \frac{Ln\,x}{cosh^2\,x} dx\ = I'(0) = Ln(\pi/4) - \gamma\ . \tag{16}$$

Accordingly, Eq. (3) may be simplified to

$$\int_0^{\frac{\beta_C\omega_D}{2}} dx\ \frac{tanh\,(x)}{x}\ = Ln\left(\frac{\beta_C\,\omega_D}{2}\right) tanh\left(\frac{\beta_C\,\omega_D}{2}\right) - Ln\left(\frac{\pi}{4}\right) + \gamma\ . \tag{17}$$

As before, the weak-coupling limit ($\beta_c\ \omega_D \gg 1$) enables us to take the hyperbolic tangent in Eq. (17) to be unity, we are therefore left with

$$\int_0^{\frac{\beta_C\omega_D}{2}} dx\ \frac{tanh\,(x)}{x}\ = Ln\left(\frac{\beta_C\,\omega_D}{2}\right) - Ln\left(\frac{\pi}{4}\right) + \gamma\ . \tag{18}$$

By grouping all factors in one Logarithmic term, we obtain

$$\int_0^{\frac{\beta_C\omega_D}{2}} dx\ \frac{tanh\,(x)}{x}\ = Ln\left(\frac{2\,e^{\gamma}}{\pi}\ \ \beta_c\ \omega_D\right)\quad . \tag{19}$$

Numerically we get, to five decimal places,

$$\frac{2\,e^{\gamma}}{\pi} = 1.13387 \tag{20}$$

so that we finally reach the conclusion

$$\int_0^{\frac{\beta_c\omega_D}{2}} dx\, \frac{tanh\,(x)}{x} = Ln(1.13387\;\beta_c\,\omega_D)\,; \qquad \beta_c\omega_D \gg 1\;. \tag{21}$$

2. Objective

From previous section we see that to obtain the result, Eq. (21), by analytic method one must encounter pretty tedious work that requires several tricks including some familiarity with Gamma and Dirichlet Eta functions and their derivatives. Now we present another method that requires no such difficulties, employing both simple analytic and numerical techniques. Numerical part participates in finding the optimum point to get the results converged. We call it "numerical convergence method". We shall see in the last section that its result is numerically equivalent to the analytic method that we mentioned earlier.

3. Methodology

The idea of numerical convergence method is simple. Let us focus on the integrand. In order to simplify the integral $\int_0^{\frac{\beta_c\omega_D}{2}} dx\, \frac{tanh\,(x)}{x}$ we define a new discontinuous function

$$g_{\tilde{x}}(x) \equiv \begin{cases} tanh(x) & ;0 < x \le \tilde{x} \\ 1 & ;x > \tilde{x} \end{cases}, \tag{22}$$

where we have approximated $tanh(x)$ by $g_{\tilde{x}}(x)$, realizing that the hyperbolic tangent function asymptotically tends to unity. By this, we have adopted the parameter $\tilde{x}$ after which $g_{\tilde{x}}(x)$ becomes unity. This parameter is, of course, adjustable.

After replacing $tanh(x)$ by $g_{\tilde{x}}(x)$, we can simply evaluate the integral $\int_0^{\frac{\beta_c\omega_D}{2}} dx\, \frac{tanh\,(x)}{x}$ and obtain

$$\int_0^{\frac{\beta_c\omega_D}{2}} \frac{tanh\,(x)}{x}\; dx \cong \int_0^{\tilde{x}} \frac{tanh\,(x)}{x}\; dx + \int_{\tilde{x}}^{\frac{\beta_c\omega_D}{2}} \frac{1}{x}\; dx. \tag{23}$$

The advantage is that the second integral on the RHS can be simply carried out, yielding

$$\int_0^{\frac{\beta_c\omega_D}{2}} \frac{tanh\,(x)}{x}\,dx \cong \int_0^{\tilde{x}} \frac{tanh\,(x)}{x}\,dx + Ln\left(\frac{\beta_c\omega_D}{2\tilde{x}}\right) \quad . \qquad (24)$$

Two terms on the right maybe grouped in a single one under the Logarithmic expression, *i.e.*,

$$\int_0^{\frac{\beta_c\omega_D}{2}} \frac{tanh\,(x)}{x}\,dx \cong Ln\left(\beta_c\omega_D\left(\frac{Exp\left[\int_0^{\tilde{x}} \frac{tanh\,(x)}{x}\,dx\right]}{2\tilde{x}}\right)\right). \qquad (25)$$

This equation may be rewritten as

$$\int_0^{\frac{\beta_c\omega_D}{2}} \frac{tanh\,(x)}{x}\,dx \cong Ln\,(\beta_c\omega_D\Phi(\tilde{x}))\ , \qquad (26)$$

provided that we define the function $\Phi(\tilde{x})$ such that

$$\Phi(\tilde{x}) \equiv \frac{Exp\left[\int_0^{\tilde{x}} \frac{tanh\,(x)}{x}\,dx\right]}{2\tilde{x}}. \qquad (27)$$

The main idea of this method is to find suitable values of $\tilde{x}$ that makes $\Phi(\tilde{x})$ numerically convergent, up to 5 decimal places of accuracy.

4. Results

In order to see the convergence of $\Phi(\tilde{x})$, we input several numerical values of x_c and evaluate $\int_0^{\tilde{x}} \frac{tanhx}{x}dx$, $exp\left\{\int_0^{\tilde{x}} \frac{tanhx}{x}dx\right\}$, and then Φ . All numerical values are displayed in 5 decimal places. the results are given in Table 1.

Table 1 Numerical values of Φ for some values of $\tilde{x}$ (calculated with Mathematica 10)

$\tilde{x}$	$\int_0^{\tilde{x}} \frac{tanhx}{x}dx$	$exp\left\{\int_0^{\tilde{x}} \frac{tanhx}{x}dx\right\}$	$\Phi \equiv \frac{exp\left\{\int_0^{\tilde{x}} \frac{tanhx}{x}dx\right\}}{2\tilde{x}}$
1.0	0.90968	2.48351	1.24176
2.0	1.51941	4.56954	1.14238
3.0	1.91811	6.80809	1.13468
4.0	2.20515	9.07161	1.13395
5.0	2.42823	11.3388	1.13388
6.0	2.61054	13.6064	1.13387

$\tilde{x}$	$\int_0^{\tilde{x}} \frac{tanhx}{x} dx$	$exp\left\{\int_0^{\tilde{x}} \frac{tanhx}{x} dx\right\}$	$\Phi \equiv \frac{exp\left\{\int_0^{\tilde{x}} \frac{tanhx}{x} dx\right\}}{2\tilde{x}}$
7.0	2.76469	15.8741	1.13387
8.0	2.89822	18.1419	1.13387
9.0	3.01600	20.4096	1.13387
10.0	3.12137	22.6773	1.13387

5. Conclusions and Discussions

As obviously seen from Table 1, the numerical value converges at Φ = 1.13387. Even though we don't exactly identify the onset of real $\tilde{x}$ that makes Φ converged, we pay attention on integral numbers of $\tilde{x}$ instead and find that Φ converges at $\tilde{x} = 6.0$ onwards.

With this, Eq. (26) turns out to be, for $\beta_c\omega_D \gg 1$,

$$\int_0^{\frac{\beta_c\omega_D}{2}} \frac{tanh\,(x)}{x} \; dx \cong Ln\,(1.13387\;\beta_c\omega_D) \tag{28}$$

which is obviously equivalent to that obtained from analytic method, Eq. (21) in introduction section. We have to emphasize that in analytic method we deal with cumbersome derivations and we unavoidably confront Dirichlet Eta and Gamma functions and their derivatives. On the other hand, by numerical convergence method we just evaluate Φ at some input values of $\tilde{x}$, and after we obtain the converged value of Φ we get from Eq.(26) the correct value of $\int_0^{\frac{\beta_c\omega_D}{2}} \frac{tanh\,(x)}{x} \; dx$, which is numerically identical to $\frac{2\,e^{\gamma}}{\pi}$ obtained by analytic method.

Not surprisingly, the accuracy of this method can go beyond 5 decimal places if we set it to be. For 2 examples, to obtain converged numerical value of Φ for 8 decimal places of accuracy we have to go up to $\tilde{x} = 9.0$ onwards and get $\Phi = 1.13386592$, and in case of 10 decimal places of accuracy we have to go up to $\tilde{x} = 11.0$ onwards and obtain $\Phi = 1.1338659173$. Both are undoubtedly equal to the numerical values of $\frac{2\,e^{\gamma}}{\pi}$. The higher level of accuracy we set, the greater value of $\tilde{x}$ we employ.

Even though evaluation of Φ at accuracy levels much higher than 5 decimal places can be performed in principle but, in practice, it is pointless to go for that since researchers in this field so far pay no attention on it. They just take numerical values of $\frac{2\,e^{\gamma}}{\pi}$ for 2 decimal places. For example, some textbook authors take it to be just 1.13 (Annett, 2003; Tinkham, 2004; Fetter & Walecka, 2003; Grosso & Parravicini, 2000). Moreover, some others display it more roughly as 1.14 (Alexandrov, 2003; Kittel, 1987; Mahan, 1990).

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