The Sommerfeld Expansion
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HRW

# Appendix C

## The Sommerfeld Expansion

The Sommerfeld expansion is applied to integrals of the form

$$\int_{-\infty}^{\infty} d\mathcal{E}\, H(\mathcal{E}) f(\mathcal{E}), \quad f(\mathcal{E}) = \frac{1}{e^{(\mathcal{E}-\mu)/k_B T} + 1}, \tag{C.1}$$

where $H(\mathcal{E})$ vanishes as $\mathcal{E} \to -\infty$ and diverges no more rapidly than some power of $\mathcal{E}$ as $\mathcal{E} \to +\infty$. If one defines

$$K(\mathcal{E}) = \int_{-\infty}^{\mathcal{E}} H(\mathcal{E}')\, d\mathcal{E}', \tag{C.2}$$

so that

$$H(\mathcal{E}) = \frac{dK(\mathcal{E})}{d\mathcal{E}}, \tag{C.3}$$

then one can integrate by parts[1] in (C.1) to get

$$\int_{-\infty}^{\infty} H(\mathcal{E}) f(\mathcal{E})\, d\mathcal{E} = \int_{-\infty}^{\infty} K(\mathcal{E}) \left( -\frac{\partial f}{\partial \mathcal{E}} \right) d\mathcal{E}. \tag{C.4}$$

Since $f$ is indistinguishable from zero when $\mathcal{E}$ is more than a few $k_B T$ greater than $\mu$, and indistinguishable from unity when $\mathcal{E}$ is more than a few $k_B T$ less than $\mu$, its $\mathcal{E}$-derivative will be appreciable only within a few $k_B T$ of $\mu$. Provided that $H$ is nonsingular and not too rapidly varying in the neighborhood of $\mathcal{E} = \mu$, it is very reasonable to evaluate (C.4) by expanding $K(\mathcal{E})$ in a Taylor series about $\mathcal{E} = \mu$, with the expectation that only the first few terms will be of importance:

$$K(\mathcal{E}) = K(\mu) + \sum_{n=1}^{\infty} \left[ \frac{(\mathcal{E} - \mu)^n}{n!} \right] \left[ \frac{d^n K(\mathcal{E})}{d\mathcal{E}^n} \right]_{\mathcal{E}=\mu}. \tag{C.5}$$

When we substitute (C.5) in (C.4), the leading term gives just $K(\mu)$, since

$$\int_{-\infty}^{\infty} (-\partial f/\partial \mathcal{E})\, d\mathcal{E} = 1.$$

Furthermore, since $\partial f/\partial \mathcal{E}$ is an even function of $\mathcal{E} - \mu$, only terms with even $n$ in (C.5) contribute to (C.4), and if we reexpress $K$ in terms of the original function $H$ through (C.2), we find that:

$$\int_{-\infty}^{\infty} d\mathcal{E}\, H(\mathcal{E}) f(\mathcal{E}) = \int_{-\infty}^{\mu} H(\mathcal{E})\, d\mathcal{E} + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \frac{(\mathcal{E} - \mu)^{2n}}{(2n)!} \left( -\frac{\partial f}{\partial \mathcal{E}} \right) d\mathcal{E}\, \frac{d^{2n-1}}{d\mathcal{E}^{2n-1}} H(\mathcal{E})\Big|_{\mathcal{E}=\mu}. \tag{C.6}$$

[1] The integrated term vanishes at $\infty$ because the Fermi function vanishes more rapidly than $K$ diverges, and at $-\infty$ because the Fermi function approaches unity while $K$ approaches zero.

Finally, making the substitution $(\mathcal{E} - \mu)/k_B T = x$, we find that

$$\int_{-\infty}^{\infty} H(\mathcal{E}) f(\mathcal{E})\, d\mathcal{E} = \int_{-\infty}^{\mu} H(\mathcal{E})\, d\mathcal{E} + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \frac{d^{2n-1}}{d\mathcal{E}^{2n-1}} H(\mathcal{E})\big|_{\mathcal{E}=\mu}, \tag{C.7}$$

where the $a_n$ are dimensionless numbers given by

$$a_n = \int_{-\infty}^{\infty} \frac{x^{2n}}{(2n)!} \left( -\frac{d}{dx} \frac{1}{e^x + 1} \right) dx. \tag{C.8}$$

By elementary manipulations one can show that

$$a_n = 2\left(1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \frac{1}{5^{2n}} - \cdots \right). \tag{C.9}$$

This is usually written in terms of the Riemann zeta function, $\zeta(n)$, as

$$a_n = \left(2 - \frac{1}{2^{2(n-1)}}\right) \zeta(2n), \tag{C.10}$$

where

$$\zeta(n) = 1 + \frac{1}{2^n} + \frac{1}{3^n} + \frac{1}{4^n} + \cdots. \tag{C.11}$$

For the first few $n$, $\zeta(2n)$ has the values[2]

$$\zeta(2n) = 2^{2n-1} \frac{\pi^{2n}}{(2n)!} B_n \tag{C.12}$$

where the $B_n$ are known as Bernoulli numbers, and

$$B_1 = \frac{1}{6}, \quad B_2 = \frac{1}{30}, \quad B_3 = \frac{1}{42}, \quad B_4 = \frac{1}{30}, \quad B_5 = \frac{5}{66}. \tag{C.13}$$

In most practical calculations in metals physics, one rarely needs to know more than $\zeta(2) = \pi^2/6$, and never goes beyond $\zeta(4) = \pi^4/90$. Nevertheless, if one should wish to carry the Sommerfeld expansion (2.70) beyond $n = 5$ (and hence past the values of the $B_n$ listed in (C.13)), by the time $2n$ is as large as 12 the $a_n$ can be evaluated to five-place accuracy by retaining only the first two terms in the alternating series (C.9).

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[2] See, for example, E. Jahnke and F. Emde, *Tables of Functions*, 4th ed., Dover, New York, 1945, p. 272.