Sommerfeld Expansion

Phy-801

February 2026

1 Introduction

Sommerfeld also provided a useful calculation tool. Many observables in Sommerfeld's theory take the form of integrals of the form

$$L(T,\mu) = \int_{-\infty}^{\infty} d\varepsilon\, \lambda(\varepsilon) f_{\rm FD}(\beta(\varepsilon-\mu)) \tag{1}$$

where $\beta = (k_{\rm B}T)^{-1}$ and $f_{\rm FD} = (e^x+1)^{-1}$ and $\lambda(\varepsilon)$ is some function of energy, generically of the form $\lambda(\varepsilon) = \ell(\varepsilon)g(\varepsilon)$ where $g(\varepsilon)$ is the density of states and $\ell(\varepsilon)$ some integrand.

Sommerfeld showed that this expanded as a power series in the temperature T

$$\begin{aligned} L(T,\mu) &= \int_{-\infty}^{\mu} d\varepsilon\, \lambda(\varepsilon) + 2\sum_{n=1}^{\infty}(1-2^{1-2n})\zeta(2n)(k_{\rm B}T)^{2n}\lambda^{(2n-1)}(\mu) \\ &= \int_{-\infty}^{\mu} d\varepsilon \lambda(\varepsilon) + \tfrac{1}{6}(\pi k_{\rm B}T)^2\lambda'(\mu) + \tfrac{7}{360}(\pi k_{\rm B}T)^4\lambda^{(3)}(\mu) + O(k_{\rm B}T)^6 \end{aligned}, \tag{2}$$

where $\lambda^{(n)}(\mu) = \frac{d^n}{d\varepsilon^n}\lambda(\varepsilon)\big|_{\varepsilon=\mu}$.

At fixed electron number density n it is further necessary to account for the temperature variation of μ. One may obtain the chemical potential as a power series in T

$$\mu(T) = \varepsilon_{\rm F} - \tfrac{1}{6}(\pi k_{\rm B}T)^2\frac{g'_{\rm F}}{g_{\rm F}} + O(k_{\rm B}T)^4 \tag{3}$$

where $g(\varepsilon)$ is the density of states and $g_{\rm F}^{(n)} = \frac{d^n}{d\varepsilon^n}g(\varepsilon)\big|_{\varepsilon=\varepsilon_{\rm F}}$ and $\varepsilon_{\rm F} = \mu(T=0)$ where higher order corrections may be straightforwardly calculated, but are not presented here. Substituting the power series form of $\mu(T)$ into (2) yields an expansion of L at fixed number density n in terms of derivatives at the fermi energy which is most succinctly expressed in terms of $\ell(\varepsilon)$

$$\begin{aligned} L(T,\mu(T)) &= \int_{-\infty}^{\varepsilon_{\rm F}} d\varepsilon\lambda(\varepsilon) + \tfrac{1}{6}(\pi k_{\rm B}T)^2\left(\frac{g_{\rm F}\lambda'_{\rm F} - g'_{\rm F}\lambda_{\rm F}}{g_{\rm F}}\right) + O(k_{\rm B}T)^4 \\ &= \int_{-\infty}^{\varepsilon_{\rm F}} d\varepsilon g(\varepsilon)\ell(\varepsilon) + \tfrac{1}{6}(\pi k_{\rm B}T)^2 g_{\rm F}\ell'_{\rm F} + O(k_{\rm B}T)^4. \\ &= L(0,\varepsilon_{\rm F}) + \tfrac{1}{6}(\pi k_{\rm B}T)^2 g_{\rm F}\ell'_{\rm F} + O(k_{\rm B}T)^4. \end{aligned} \tag{4}$$

In this note (a large portion of which is lifted from Ashcroft and Mermin Appendix C), we derive this power series.

2 Sommerfeld expansion

The Sommerfeld expansion is applied to integrals of the form

$$L = \int_{-\infty}^{\infty} d\varepsilon\, \lambda(\varepsilon) f(\varepsilon), \qquad f(\varepsilon) = f_{\rm FD}(\beta(\varepsilon-\mu)) = \frac{1}{e^{(\varepsilon-\mu)/k_{\rm B}T}+1}, \tag{5}$$

where $\lambda(\varepsilon)$ vanishes as $\varepsilon \to -\infty$ and diverges no more rapidly than some power of ε as $\varepsilon \to +\infty$. If one defines

$$\Lambda(\varepsilon) = \int_{-\infty}^{\varepsilon} \lambda(\varepsilon')\, d\varepsilon', \tag{6}$$

so that

$$\lambda(\varepsilon) = \frac{d\Lambda(\varepsilon)}{d\varepsilon}, \tag{7}$$

then one can integrate by parts in (5) to get

$$\int_{-\infty}^{\infty} \lambda(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\infty} \Lambda(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon. \tag{8}$$

Since f is indistinguishable from zero when ε is more than a few $k_{\rm B}T$ greater than μ, and indistinguishable from unity when ε is more than a few $k_{\rm B}T$ less than μ, its ε-derivative will be appreciable only within a few $k_{\rm B}T$ of μ. Provided that λ is nonsingular and not too rapidly varying in the neighborhood of $\varepsilon = \mu$, it is very reasonable to evaluate (8) by expanding $\Lambda(\varepsilon)$ in a Taylor series about $\varepsilon = \mu$, with the expectation that only the first few terms will be of importance:

$$\Lambda(\varepsilon) = \Lambda(\mu) + \sum_{n=1}^{\infty} \frac{(\varepsilon-\mu)^n}{n!} \left.\frac{d^n \Lambda(\varepsilon)}{d\varepsilon^n}\right|_{\varepsilon=\mu}. \tag{9}$$

When we substitute (9) in (8), the leading term gives just $\Lambda(\mu)$, since

$$\int_{-\infty}^{\infty} \left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon = 1. \tag{10}$$

Furthermore, since $\partial f/\partial \varepsilon$ is an even function of $\varepsilon - \mu$, only terms with even n in (9) contribute to (8), and if we reexpress Λ in terms of the original function λ through (6), we find that

$$\int_{-\infty}^{\infty} d\varepsilon\, \lambda(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} \lambda(\varepsilon)\, d\varepsilon + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \frac{(\varepsilon-\mu)^{2n}}{(2n)!} \left(-\frac{\partial f}{\partial \varepsilon}\right) \left.\frac{d^{2n-1}}{d\varepsilon^{2n-1}} \lambda(\varepsilon)\right|_{\varepsilon=\mu}. \tag{11}$$

Finally, making the substitution $(\varepsilon - \mu)/k_{\rm B}T = x$, we find that

$$\int_{-\infty}^{\infty} \lambda(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\mu} \lambda(\varepsilon)\, d\varepsilon + \sum_{n=1}^{\infty} a_n (k_{\rm B}T)^{2n} \left.\frac{d^{2n-1}}{d\varepsilon^{2n-1}} \lambda(\varepsilon)\right|_{\varepsilon=\mu}, \tag{12}$$

where the a_n are dimensionless numbers given by

$$a_n = \int_{-\infty}^{\infty} \frac{x^{2n}}{(2n)!} \left(-\frac{d}{dx}\frac{1}{e^x+1}\right) dx. \tag{13}$$

By elementary manipulations one can show that

$$a_n = 2\left(1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \frac{1}{5^{2n}} - \cdots\right). \tag{14}$$

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

$$a_n = 2\left(1 - 2^{1-2n}\right) \zeta(2n), \tag{15}$$

where

$$\zeta(n) = 1 + \frac{1}{2^n} + \frac{1}{3^n} + \frac{1}{4^n} + \cdots. \tag{16}$$

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

$$\zeta(2n) = \frac{2^{2n-1}\pi^{2n}}{(2n)!} B_n, \tag{17}$$

where the B_n are known as Bernoulli numbers, and

$$B_1 = \frac{1}{6}, \quad B_2 = \frac{1}{30}, \quad B_3 = \frac{1}{42}, \quad B_4 = \frac{1}{30}, \quad B_5 = \frac{5}{66}. \tag{18}$$

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 beyond $n = 5$ (and hence past the values of the B_n listed in (18)), 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 (14).

3 Corrections at fixed N

In a system of fixed electron number, the electron density n is independent of temperature, and instead the chemical potential μ varies with T. This variation can be calculated by considering the electron density

$$n(T, \mu) = \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon) f_{\mathrm{FD}}(\beta(\varepsilon - \mu)) \tag{19}$$

where $g(\varepsilon)$ is the density of states. Applying the result (2) we get

$$n(T, \mu) = n(0, \varepsilon_{\mathrm{F}}) + \int_{\varepsilon_{\mathrm{F}}}^{\mu} d\varepsilon g(\varepsilon) + \tfrac{1}{6}(\pi k_{\mathrm{B}} T)^2 g'(\mu) + \tfrac{7}{360}(\pi k_{\mathrm{B}} T)^4 g^{(3)}(\mu) + \cdots \tag{20}$$

where number conservation requires that the leading terms on each side cancel $n(T, \mu) = n(0, \varepsilon_{\mathrm{F}})$. Using that μ is an even function of T (this follows as n is an even function), we then expand in powers of T

$$\begin{aligned} \int_{\varepsilon_{\mathrm{F}}}^{\mu} d\varepsilon g(\varepsilon) &= \tfrac{1}{2} g(\varepsilon_{\mathrm{F}}) \mu_0^{(2)} T^2 + \ldots \\ g^{(n)}(\mu) &= g^{(n)}(\varepsilon_{\mathrm{F}}) + \tfrac{1}{2} g^{(n+1)}(\varepsilon_{\mathrm{F}}) \mu_0^{(2)} T^2 + \ldots \end{aligned} \tag{21}$$

where $\mu_0^{(n)} = \left. \frac{\partial^n \mu}{\partial T^n} \right|_{T=0}$. Inserting these expansions (21) into (20) and solving for the $\mu_0^{(n)}$ yields a power series form for the chemical potential

$$\mu(T) = \varepsilon_{\mathrm{F}} - \tfrac{1}{6}(\pi k_{\mathrm{B}} T)^2 \frac{g'(\varepsilon_{\mathrm{F}})}{g(\varepsilon_{\mathrm{F}})} - \ldots. \tag{22}$$

Subsequently inserting this into (2) yields (4).