

Appendix A

The Proof of $G_{even}^{weak}(V)$ Is an Even Function

According to (2.144),

$$G_{even}^{weak}(V) = A - B \int_{-\infty}^{\infty} \left[\int_{-E_0}^{E_0} \frac{\tanh(\frac{\epsilon'}{2k_B T})}{\epsilon' - \omega} d\epsilon' \right] \frac{\partial f(\omega - eV)}{\partial \omega} d\omega, \quad (\text{A.1})$$

$$= A - B \int_{-\infty}^{\infty} Q(\omega) \frac{\partial f(\omega - eV)}{\partial \omega} d\omega, \quad (\text{A.2})$$

for $-E_0 < \epsilon' < E_0$, where A and B are constants, and

$$Q(\omega) = \int_{-E_0}^{E_0} \frac{\tanh(\frac{\epsilon'}{2k_B T})}{\epsilon' - \omega} d\epsilon'. \quad (\text{A.3})$$

Prove that $G_{even}^{weak}(V)$ is an even function.

A.1 $Q(\omega)$ Is an Even Function

Show that $Q(\omega)$ in (A.3) is an even function with respect to ω .

Proof:

$$Q(-\omega) = \int_{-E_0}^{E_0} \frac{\tanh(\frac{\epsilon'}{2k_B T})}{\epsilon' + \omega} d\epsilon'$$

$$\begin{aligned}
&= - \int_{E_0}^{-E_0} \frac{\tanh\left(\frac{-x}{2k_B T}\right)}{-x + \omega} dx, \text{ where we let } \epsilon' = -x \\
&= - \int_{E_0}^{-E_0} \frac{\tanh\left(\frac{x}{2k_B T}\right)}{x - \omega} dx, \text{ because } \tanh\left(\frac{-x}{2k_B T}\right) = -\tanh\left(\frac{x}{2k_B T}\right) \\
&= \int_{-E_0}^{E_0} \frac{\tanh\left(\frac{x}{2k_B T}\right)}{x - \omega} dx, \\
&= Q(\omega), \text{ Q. E. D.} \tag{A.4}
\end{aligned}$$

A.2 $G_{even}^{weak}(V)$ Is an Even Function

Show that $G_{even}^{weak}(V)$ in (A.2) is an even function with respect to V .

Proof:

According to (A.2), $G_{even}^{weak}(V)$ can be written as

$$\begin{aligned}
G_{even}^{weak}(V) &= A + B \int_{-\infty}^{\infty} Q(\omega) \frac{\beta e^{\beta(\omega-eV)}}{[1 + e^{\beta(\omega-eV)}]^2} d\omega, \text{ where } \beta = \frac{1}{k_B T} \\
&= A + B \int_{-\infty}^{\infty} Q(\omega) \frac{\beta}{[e^{-\beta(\omega-eV)/2} + e^{\beta(\omega-eV)/2}]^2} d\omega. \tag{A.5}
\end{aligned}$$

Therefore,

$$\begin{aligned}
G_{even}^{weak}(-V) &= A + B \int_{-\infty}^{\infty} Q(\omega) \frac{\beta}{[e^{-\beta(\omega+eV)/2} + e^{\beta(\omega+eV)/2}]^2} d\omega \\
&= A - B \int_{\infty}^{-\infty} Q(-x) \frac{\beta}{[e^{-\beta(-x+eV)/2} + e^{\beta(-x+eV)/2}]^2} dx, \\
&\hspace{15em} \text{where we let } \omega = -x \\
&= A - B \int_{\infty}^{-\infty} Q(x) \frac{\beta}{[e^{\beta(x-eV)/2} + e^{-\beta(x-eV)/2}]^2} dx, \\
&\hspace{15em} \text{because } Q(-\omega) = Q(\omega) \text{ as shown in (A.4)} \\
&= A + B \int_{-\infty}^{\infty} Q(x) \frac{\beta}{[e^{\beta(x-eV)/2} + e^{-\beta(x-eV)/2}]^2} dx. \tag{A.6}
\end{aligned}$$

Compare (A.5) and (A.6), we have $G_{even}^{weak}(-V) = G_{even}^{weak}(V)$. Q. E. D.

Appendix B

Simpson's Rule and Composite Simpson's Rule

In numerical analysis, Simpson's rule is a method for numerical integration. Specifically, it is the following approximation:

$$\int_a^b f(x)dx \approx \frac{b-a}{6} [f(a) + 4f(\frac{a+b}{2}) + f(b)], \text{ for a small interval } [a, b] \quad (\text{B.1})$$

But, if the interval $[a, b]$ is not small, we can divide it into n small intervals, where n is an even number, as shown in Fig. B.1. Let $h = (b-a)/n$, and then the integration can be approximated as

$$\begin{aligned} \int_a^b f(x)dx &\approx \frac{2h}{6} \{ [f(x_0) + 4f(x_1) + f(x_2)] + [f(x_2) + 4f(x_3) + f(x_4)] + \dots \} \\ &= \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \dots \\ &\quad + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] \\ &= \frac{h}{3} [f(x_0) + 4 \sum_{j=0}^{\frac{n}{2}-1} f(x_{2j+1}) + 2 \sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + f(x_n)] \end{aligned} \quad (\text{B.2})$$

The approximation (B.2) is called composite Simpson's rule and can be calculated using computer programs.

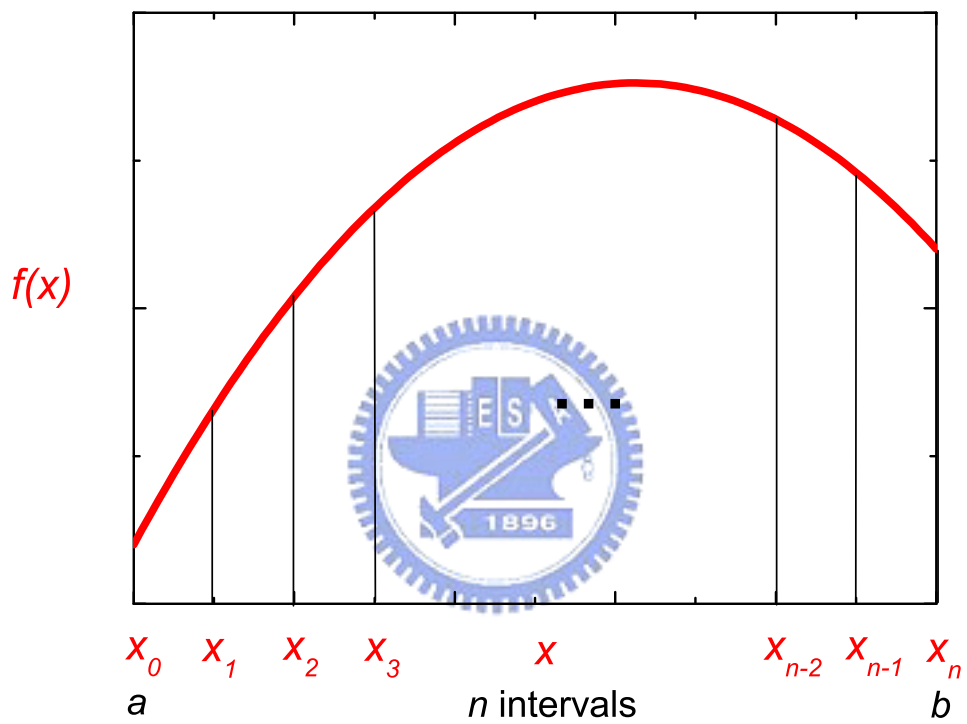


Figure B.1: The composite Simpson's rule.