4.2: Legendre Transforms

The microcanonical ensemble involved the thermodynamic variables N, V and E as its variables. However, it is often convenient and desirable to work with other thermodynamic variables as the control variables. Legendre transforms provide a means by which one can determine how the energy functions for different sets of thermodynamic variables are related. The general theory is given below for functions of a single variable.

Consider a function $f(x)$ and its derivative

$$y = f'(x) = \frac{df}{dx} \equiv g(x)$$

The equation $y = g(x)$ defines a *variable transformation* from x to y. Is there a unique description of the function $f(x)$ in terms of the variable y? That is, does there exist a function $\phi(y)$ that is equivalent to $f(x)$?

Given a point x_0, can one determine the value of the function $f(x_0)$ given only $f'(x_0)$? No, for the reason that the function $f(x_0) + c$ for any constant c will have the same value of $f'(x_0)$ as shown in Figure $4.2.1$.

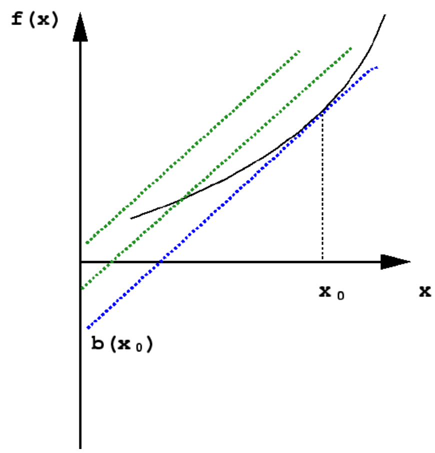

Figure $4.2.1$: The Legendre transfer in action (Mark Tuckerman)

However, the value $f(x_0)$ can be determined uniquely if we specify the slope of the line tangent to f at x_0, i.e., $f'(x_0)$ and the y-intercept, $b(x_0)$ of this line. Then, using the equation for the line, we have

$$f(x_0) = x_0 f'(x_0) + b(x_0)$$

This relation must hold for any general x:

$$f(x) = x f'(x) + b(x)$$

Note that $f'(x)$ is the variable y, and $x = g^{-1}(y)$, where g_{-1} is the functional inverse of g, i.e., $g(g^{-1}(x)) = x$. Solving for $b(x) = b(g^{-1}(y))$ gives

$$b(g^{-1}(y)) = f(g^{-1}(y)) - y g^{-1}(y) \equiv \phi(y)$$

where $\phi(y)$ is known as the **Legendre transform** of $f(x)$. In shorthand notation, one writes

$$\phi(y) = f(x) - xy$$

however, it must be kept in mind that x is a function of y.