Jacobian Technique

Suppose we need to find the heat capacity at constant volume (and total number of particles) of a quantum gas:

\[ C_V = T \left( \frac{\partial S}{\partial T} \right)_{V,N} \]  

(1)

To explicitly do the partial derivative (1) we need to know an analytic expression for \( S \) as a function of \( N, V, \) and \( T. \) [Otherwise we will need to do the derivative numerically, which is quite possible, but rather cumbersome.] Our results for quantum gases are obtained in the grand canonical formalism where the natural variables are \( (T, \mu, V) \), rather than \( (T, N, V) \). There is a generic technique for solving problems like that based on the properties of Jacobians.

Suppose we have \( m \) functions, \( y_1, y_2, \ldots, y_m \), of \( m \) variables, \( x_1, x_2, \ldots, x_m \). If we introduce the matrix \( M \) as

\[ M_{ij} = \frac{\partial y_i}{\partial x_j}, \]  

(2)

then, by definition, the Jacobian of the given set of functions and arguments is the determinant of \( M \):

\[ \frac{\partial (y_1, y_2, \ldots, y_m)}{\partial (x_1, x_2, \ldots, x_m)} = \det M. \]  

(3)

[The left-hand side of (3) is the symbol for corresponding Jacobian.]

Now we mention some important properties of Jacobians. The first property immediately follows from the definition:

\[ \frac{\partial (x_1, x_2, \ldots, x_m)}{\partial (x_1, x_2, \ldots, x_m)} \equiv 1. \]  

(4)

The most crucial property is:

\[ \frac{\partial (y_1, y_2, \ldots, y_m)}{\partial (z_1, z_2, \ldots, z_m)} \cdot \frac{\partial (z_1, z_2, \ldots, z_m)}{\partial (x_1, x_2, \ldots, x_m)} = \frac{\partial (y_1, y_2, \ldots, y_m)}{\partial (x_1, x_2, \ldots, x_m)}. \]  

(5)

One readily gets Eq. (5) from the chain rule for partial derivatives,

\[ \frac{\partial y_i}{\partial x_j} = \sum_{k=1}^{m} \frac{\partial y_i}{\partial z_k} \frac{\partial z_k}{\partial x_j}, \]  

(6)

and the theorem that the determinant of a product of matrices—the right-hand side of Eq. (6) is nothing else than the product of matrices—is equal to the product of their determinants.

With (4) and (5), we obtain

\[ \frac{\partial (y_1, y_2, \ldots, y_m)}{\partial (x_1, x_2, \ldots, x_m)} \cdot \frac{\partial (x_1, x_2, \ldots, x_m)}{\partial (y_1, y_2, \ldots, y_m)} = 1, \]  

(7)

that is

\[ \frac{\partial (x_1, x_2, \ldots, x_m)}{\partial (y_1, y_2, \ldots, y_m)} = \left[ \frac{\partial (y_1, y_2, \ldots, y_m)}{\partial (x_1, x_2, \ldots, x_m)} \right]^{-1}. \]  

(8)

We see that formal behavior of Jacobians is reminiscent of the algebraic behavior of fractions. It is also worth mentioning that if we interchange any two functions in the “numerator”, then the Jacobian changes its sign, the same is true for any two arguments in the “denominator”, both properties being obvious, since determinants change signs when any two columns/rows are exchanged.
Why Jacobians are good for our purposes? Because of the following formula (readily seen from the definition):

\[ \frac{\partial(u, x_2, \ldots, x_m)}{\partial(x_1, x_2, \ldots, x_m)} = \left( \frac{\partial u}{\partial x_1} \right)_{x_2, \ldots, x_m}. \tag{9} \]

**Example.** Consider Eq. (1). We can write it as

\[ C_V = T \frac{\partial(S, N)}{\partial(T, N)}. \tag{10} \]

[Note that I do not include \( V \) in the Jacobian, since with respect to the quantity and variables of interest, the variable \( V \) plays a role of a fixed external parameter which does not participate in the transformation of variables.—The situation would be different for \( C_P \).]

We write

\[ \frac{\partial(S, N)}{\partial(T, N)} = \frac{\partial(S, N)}{\partial(T, \mu)} \cdot \frac{\partial(T, \mu)}{\partial(T, N)} = \frac{\partial(S, N)}{\partial(T, \mu)} \cdot \left[ \frac{\partial(T, N)}{\partial(T, \mu)} \right]^{-1} = \frac{\partial(S, N)}{\partial(T, \mu)} \cdot \frac{\partial N}{\partial \mu}_{T,V}. \tag{11} \]

By definition,

\[ \frac{\partial(S, N)}{\partial(T, \mu)} = \left( \frac{\partial S}{\partial T} \right)_{V,\mu} \left( \frac{\partial N}{\partial \mu} \right)_{V,T} - \left( \frac{\partial N}{\partial T} \right)_{V,\mu} \left( \frac{\partial S}{\partial \mu} \right)_{V,T}. \tag{12} \]

It is also reasonable to take into account the Maxwell-type relation

\[ \left( \frac{\partial N}{\partial T} \right)_{V,\mu} = \left( \frac{\partial S}{\partial \mu} \right)_{V,T}. \tag{13} \]

Finally, we get

\[ C_V = T \left( \frac{\partial S}{\partial T} \right)_{V,\mu} - T \left[ \left( \frac{\partial N}{\partial T} \right)_{V,\mu} \right]^2 / \left( \frac{\partial N}{\partial \mu} \right)_{T,V}. \tag{14} \]

**Problem 44.** Express the heat capacity at constant pressure (and total number of particles), \( C_P \), in terms of partial derivatives of \( S, P, \) and \( N \) as functions of the three grand-canonical variables \( (T, \mu, V) \).