

An Expert Path Through a Thermo Maze

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Abstract. Several studies in recent years have demonstrated that upper-division students struggle with partial derivatives and the complicated chain rules ubiquitous in thermodynamics. We asked several experts (primarily faculty who teach thermodynamics) to solve a challenging and novel thermodynamics problem in order to understand how they navigate through this maze. What we found was a tremendous variety in solution strategies and sense-making tools, both within and between individuals. This case study focuses on one particular expert: his solution paths, use of sense-making tools, and comparison of different approaches.

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INTRODUCTION

Several studies in recent years have demonstrated that students struggle to connect the mathematics and physics in thermodynamics (*e.g.* [1, 2]). One particular area of difficulty is the sea of partial derivatives and complicated chain rules ubiquitous in thermodynamics. [3, 4, 5]

This paper represents the first piece of a larger study designed to better understand why students struggle so much with the mathematics of thermodynamics, how practicing physicists deal with the mathematics of thermodynamics, and ultimately how to facilitate an appropriate transition from student to professional in this area. Towards this end, we interviewed several faculty members who teach thermodynamics and asked them to solve a challenging problem. We also presented the same problem to junior physics majors who had just completed the *Paradigms in Physics: Energy and Entropy* course. [6]

A startling aspect of this set of data is that each interviewee introduced at least one new approach or problem-solving tool. While there was some overlap, no two people took the same path through the problem or used the same set of physical and mathematical sense-making tools. However, we have begun to identify some key branch points that appear to distinguish between possible paths. This descriptive case study focuses on one particular expert, J, a senior faculty member who has taught thermodynamics multiple times. His interview explicitly highlights a few of these branch points.

The next section presents J's initial path to a solution, including various instances of sense-making, detours, and dead ends. The following section outlines two other approaches that J discussed and his reflections on how they compared to his initial approach. The final section situates this case within the larger study. The poster accompanying this paper provides a visual representation of this maze and J's journey through it. [7]

NAVIGATING THE MAZE

On a whiteboard, J was given the equations of state for a van der Waals gas,

$$p = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2} \quad (1)$$

$$S = Nk \left\{ \ln \left[\frac{(V - Nb)T^{3/2}}{N\Phi} \right] + \frac{5}{2} \right\} \quad (2)$$

$$U = \frac{3}{2}NkT - \frac{aN^2}{V}, \quad (3)$$

and asked to find

$$\left(\frac{\partial U}{\partial p} \right)_S.$$

We suggest that the reader take a few moments to consider how they might approach the problem.

J began by assuming that N was fixed and subsequently included N in the subscripts for every partial derivative. He then did some sense-making about the type of question being asked:

“When I think about these kind of relations... it's like a response function. You simply say, alright, I'm changing one variable, keeping two other variables constant. We have a system here with three independent variables... so, we have a choice here [points to p , S , and N] and then measure the change in something else [points to U].”

He identified T and V as the variables changing in Eq. 3. However, instead of using this equation of state, he chose to start from the thermodynamic identity (1st Law):

$$dU = T dS - p dV + \mu dN. \quad (4)$$

To obtain the partial derivative he wanted, J divided the whole equation by dp and set $dS = 0$ and $dN = 0$ since S and N were to be held constant:

$$\left(\frac{\partial U}{\partial p}\right)_{S,N} = -p \left(\frac{\partial V}{\partial p}\right)_{S,N}. \quad (5)$$

J pointed out that constant entropy was “always a nasty one to deal with” and that he would prefer to “have S as a changing variable, as a dependent variable [rather] than as an independent variable.” Thus, he began to look for partial derivatives that could be directly obtained from the equation of state (Eqs. 1–3) as they were given, which would eliminate the need to consider constant entropy.

His first attempt was to use the cyclic chain rule on the left side of Eq. 5:

$$\left(\frac{\partial U}{\partial p}\right)_{S,N} = - \left(\frac{\partial U}{\partial S}\right)_{p,N} \left(\frac{\partial S}{\partial p}\right)_{U,N}. \quad (6)$$

Noticing that this shifted U to be the variable held constant in $\left(\frac{\partial S}{\partial p}\right)_{U,N}$, J decided that this was a dead end and that he actually wanted to shift the dependent variable to be T , since the equations of state were given in terms of changing T and V .

Before pursuing this avenue, J briefly contemplated the physics of Eq. 5—identifying $\left(\frac{\partial V}{\partial p}\right)_{S,N}$ as the adiabatic compressibility.

He then reconsidered whether using the energy equation of state would have been easier. However, seeing that that route would involve two derivatives instead of one, he decided to move forward with his original plan.

His second attempt involved using the cyclic chain rule on the right side of Eq. 5:

$$\left(\frac{\partial V}{\partial p}\right)_{S,N} = - \left(\frac{\partial V}{\partial S}\right)_{p,N} \left(\frac{\partial S}{\partial p}\right)_{V,N}, \quad (7)$$

After inverting the first term,

$$\left(\frac{\partial V}{\partial S}\right)_{p,N} = \left[\left(\frac{\partial S}{\partial V}\right)_{p,N} \right]^{-1}, \quad (8)$$

he realized that temperature was still not present and decided to “save this step [cyclic chain rule] for later.”

Returning to the right side of Eq. 5, J chose to do a simple change of variables to introduce T as a variable:

$$\left(\frac{\partial V}{\partial p}\right)_{S,N} = \left(\frac{\partial V}{\partial T}\right)_{S,N} \left(\frac{\partial T}{\partial p}\right)_{S,N}. \quad (9)$$

Satisfied that he was on the right track, J looked for what he called “nice sets.” When asked what he meant by a “nice set,” he responded that since all of the equations of

state (Eqs. 1–3) were given in terms of the independent variables V , T , and N , a “nice set” would be a partial derivative with respect to one of these variables, with the other two held constant.

To express $\left(\frac{\partial V}{\partial T}\right)_{S,N}$ in terms of “nice sets,” he returned to his earlier detour, the cyclic chain rule he had “saved for later” (Eq. 7):

$$\begin{aligned} \left(\frac{\partial V}{\partial T}\right)_{S,N} &= - \left(\frac{\partial V}{\partial S}\right)_{T,N} \left(\frac{\partial S}{\partial T}\right)_{V,N} \\ &= - \left(\frac{\partial S}{\partial V}\right)_{T,N}^{-1} \left(\frac{\partial S}{\partial T}\right)_{V,N}. \end{aligned} \quad (10)$$

Each of these partial derivatives was now a “nice set” and thus, Eq. 5 became

$$\begin{aligned} \left(\frac{\partial U}{\partial p}\right)_{S,N} &= -p \left(\frac{\partial V}{\partial p}\right)_{S,N} \\ &= +p \left(\frac{\partial S}{\partial V}\right)_{T,N}^{-1} \left(\frac{\partial S}{\partial T}\right)_{V,N} \left(\frac{\partial T}{\partial p}\right)_{S,N} \end{aligned} \quad (11)$$

and only $\left(\frac{\partial T}{\partial p}\right)_{S,N}$ remained to be expressed in terms of “nice sets.”

In order to deal with this final factor, J used the cyclic chain rule again “to bring the S inside”

$$\left(\frac{\partial T}{\partial p}\right)_{S,N} = - \left(\frac{\partial T}{\partial S}\right)_{p,N} \left(\frac{\partial S}{\partial p}\right)_{T,N}, \quad (12)$$

but recognized that he really wanted to replace p by V in order to get another “nice set.” This realization prompted him to do a second change of variables:

$$\left(\frac{\partial T}{\partial p}\right)_{S,N} = \left(\frac{\partial T}{\partial V}\right)_{S,N} \left(\frac{\partial V}{\partial p}\right)_{S,N}. \quad (13)$$

At this point, he noticed that when he plugged this result into Eq. 11, he would get

$$-p \left(\frac{\partial V}{\partial p}\right)_{S,N} = -p \left(\frac{\partial V}{\partial p}\right)_{S,N}, \quad (14)$$

and laughingly responded, “we’re going in circles.”

J then cataloged the tools he had already used:

- change of variables (e.g. Eqs. 9, 13) and
- cyclic chain rule (e.g. Eqs. 6, 7, 10, 12).

He identified a third tool, a variant of the 2-dimensional chain rule, which he called “another kind of change of variables.” Here one splits the derivative into two terms: one with volume explicitly held constant and one where volume could be changing. He inverted the final factor in Eq. 11 and then incorrectly wrote the change of variables,

$$\left(\frac{\partial p}{\partial T}\right)_{S,N} = \left(\frac{\partial p}{\partial T}\right)_{V,N} + \left(\frac{\partial p}{\partial V}\right)_{T,N} \left(\frac{\partial V}{\partial S}\right)_{T,N}. \quad (15)$$

After inverting $\left(\frac{\partial V}{\partial S}\right)_{T,N}$, he saw that all of the partial derivatives could be calculated directly from Eqs. 1–3 and he moved on to reflect on other approaches.

However, as just mentioned, his final change of variables (Eq. 15) was written incorrectly, reversing S and T in the last partial derivative. A correct change of variables

$$\left(\frac{\partial p}{\partial T}\right)_{S,N} = \left(\frac{\partial p}{\partial T}\right)_{V,N} + \left(\frac{\partial p}{\partial V}\right)_{T,N} \left(\frac{\partial V}{\partial T}\right)_{S,N} \quad (16)$$

would require another application of Eq. 10 (cyclic chain rule) to produce a final expression in terms of “nice sets:”

$$\left(\frac{\partial U}{\partial p}\right)_{S,N} = \frac{p \left(\frac{\partial S}{\partial T}\right)_{V,N}}{\left(\frac{\partial S}{\partial V}\right)_{T,N} \left(\frac{\partial p}{\partial T}\right)_{V,N} - \left(\frac{\partial p}{\partial V}\right)_{T,N} \left(\frac{\partial S}{\partial T}\right)_{V,N}}. \quad (17)$$

Applied specifically to the van der Waals equations of state, this would yield a final answer of

$$\left(\frac{\partial U}{\partial p}\right)_{S,N} = \frac{3(V - Nb)V (aN(V - Nb) - kTV^2)}{-5kTV^3 + 6aN(V - Nb)^2}. \quad (18)$$

COMPARING OTHER ROUTES

Once J had a result in terms of partial derivatives he could find directly from the given equations of state (Eqs. 1–3), he reflected on two other paths through the problem.

Energy equation of state

During his initial solution using the thermodynamic identity, J occasionally returned to the idea of using the energy equation of state (Eq. 3) and wondered if that would have been easier. After finishing the problem, he outlined this alternate path.

J began by writing:

$$\left(\frac{\partial U}{\partial p}\right)_{S,N} = \frac{3}{2}Nk \left(\frac{\partial T}{\partial p}\right)_{S,N} + \frac{aN^2}{V^2} \left(\frac{\partial V}{\partial p}\right)_{S,N} \quad (19)$$

and noted that he really wanted the inverse of both partial derivatives on the right-hand side, since p was one of the state functions. For him, the relevant differences between this and his earlier approach were that there were now two terms instead of one and that the same tools (chain rule and change of variables) would be needed to shift S from an independent variable to a dependent variable.

At this point, J stated that Eq. 19 and Eq. 5 should be equivalent. After looking at both, he recognized that each included a $\left(\frac{\partial V}{\partial p}\right)_{S,N}$ term. He then reasoned that one

should be able to use this fact and the p equation of state (Eq. 1) to actually derive the entropy (though he didn’t remember off-hand how to do so) and “it [had] better be consistent with this equation [Eq. 2].”

Differentials

Since the *Energy and Entropy* course also uses differentials, the interviewers asked J to rework the problem using differentials, as well as to reflect on the potential utility of differentials in teaching undergraduates.

J rewrote the equations of state (Eqs. 1–3) in differential form, using blanks for some of the derivatives:

$$dU = \frac{3}{2}Nk dT + \frac{aN^2}{V^2} dV \quad (20)$$

$$dS = Nk \left(\frac{N\Phi}{V - Nb}\right) (\text{_____} dT + \text{_____} dV) \quad (21)$$

$$dp = \text{_____} dT + \text{_____} dV. \quad (22)$$

He then outlined the steps that he would use to solve this system of equations for dU in terms of dp :

1. set $dS = 0$ in Eq. 21
2. solve Eq. 21 for dV in terms of dT
3. **substitute dV into Eq. 20**
4. substitute dV into Eq. 22
5. solve Eq. 22 for dT in terms of dp
6. substitute dT into Eq. 20
7. divide Eq. 20 by dp .

In his description, J did not mention Step 3 (in bold). If this step were not included, the expression would have a $\left(\frac{\partial V}{\partial p}\right)_{S,N}$ factor. If Step 3 were included, one would obtain Eq. 18, as expected.

Comparing this method to his previous approaches, J stated he had “...never learned it this way, never thought about it this way and was never shown it,” but pointed out that “the advantage of doing it this way is that you get a system of equations, which... people know what to do with” and “this is probably more intuitive for students because... they know how to solve systems of equations.”

J also pointed out that the two formalisms (differentials and partial derivatives) were simply “a different encoding of the same information.” The primary difference he highlighted was that partial derivatives involve ratios of variables and dependent changes, where one has to be sure to choose the right ratios. In contrast, differentials involve variables and independent changes that connect to create whichever ratio is needed. Thus, depending on whether one wants to emphasize the response function, one formalism may be more appropriate than the other. He also noted that there is no other area in physics where

students encounter partial derivatives and chain rules the way that one does in thermodynamics.

THE BIRD'S EYE VIEW

The interview presented here was only one of several interviews conducted with faculty and students as they attempted to solve this problem. As of this paper, we have conducted 10 interviews with experts from several institutions and we anticipate an additional 3–5 interviews. In addition to these expert interviews, we also have 6 interviews with students and classroom data for the last several years, including activities where groups of students were working on similar problems. As mentioned earlier, each interviewee introduced new approaches and tools.

The dead ends (*e.g.* Eq. 6), detours (*e.g.* Eq. 7), and circling (*e.g.* Eq. 14) in J's initial solution, as well as the variety in solution paths and sense-making tools used by other interviewees, point to the complexity of the problem solving skills required in thermodynamics. Given this complexity, it is perhaps not surprising that students struggle so much with thermodynamics.

We are currently exploring possible theoretical and representational frameworks to model this complexity—*e.g.* cognitive task analysis [8], epistemic framing [9], cognitive blending [10], or expert/novice problem-solving [11, 12]. It is our hope that a better understanding of this complexity will allow us to better teach our students how to navigate these mazes.

Although this case study is primarily descriptive, it was chosen as a way to begin looking towards modeling the complexity of thermodynamic problem-solving. In particular, this interview highlights three branch points (briefly presented below) that appear to typify the many different paths taken in the majority of the interviews.

Which energy equation is used. J indicated that the primary difference between using the thermodynamic identity (Eq. 4) and the equation of state (Eq. 3) was in the set-up, but that both approaches must be equivalent.

Which mathematical formalism is used. One of the most notable differences involves the choice of mathematical formalism, specifically the use of partial derivatives or differentials. J summarized this difference as dealing with **ratios** of variables and **dependent** changes versus using **single** variables and **independent** changes.

How one deals with constant entropy. J demonstrated two different ways of dealing mathematically with the challenge of constant entropy:

- using chain rules to get S as a changing variable instead of a constant variable (*e.g.* Eq. 12), and
- setting $dS = 0$ in Eq. 21.

A third method used by other interviewees involved

- setting S equal to a constant in the equation of state, allowing one to relate T and V .

Almost all interviewees used one or more of these three approaches, although when they chose to use them differed. In addition, interviewees were asked to describe an experiment to measure $\left(\frac{\partial U}{\partial p}\right)_S$ and there were several ways of thinking about how one could experimentally hold the entropy constant.

In conclusion, J summarized a great deal of what we are seeing when he said:

“All of these approaches will get you there eventually, and so... what is the way that kind of makes it easier for me to organize my thoughts, in terms of finding equations?”

The different branch points, as well as J's mistakes, suggest that it would be beneficial to better understand the affordances and constraints of various paths.

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