Partial Derivatives in Thermodynamics

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An epistemological analysis of the fluidity of the definition of dependent and independent variables in thermodynamics leads to a discussion of the implications for the design and interpretation of contour diagrams in this context. An overview of research looking at expert and student calculations of partial derivatives from contour maps appropriate to thermodynamics, as part of the Paradigms in Physics project at Oregon State University, is presented, along with links to curricular materials developed in this project.

Keywords: Teaching and learning of specific topics in calculus, teachers' and students' practices related to calculus across disciplines, partial derivatives, contour diagrams, thermodynamics.

VARIABLES IN THERMODYNAMICS

Consider a series of experiments involving a gas in a piston such that the pressure p , volume V, and temperature T can be changed and/or measured, see Figure 1.

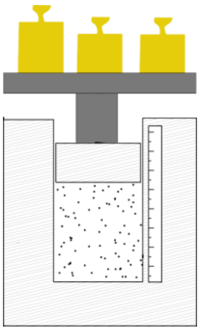

Figure 1: Gas in a piston. The pressure is controlled by adding weights to the top of the piston. The temperature is held constant by immersing the piston in a constant temperature bath or the entropy is held constant by insulating the piston (not both!).

In each run of the experiment, the temperature is held constant by immersing the piston in a constant-temperature thermal bath, which allows energy to flow into/out of the piston. The results of these experiments can be plotted as a series of isotherms on a single contour plot, see Figure 2a. Alternatively, in a series of adiabatic experiments in which the piston is insulated so that no energy flows into/out of the piston from the environment, it is the entropy S which is constant, resulting in a different contour plot, see Figure 2b. (Calculating entropy is subtle and often difficult. Holding entropy constant is easy—insulate!)

A Carnot cycle consists of a series of expansions and compressions of the piston, alternating between isothermal and adiabatic, so that the system returns to the same state, see the bold contour in Figure 2c.

In a mathematics class, the very definition of a function implies that the variables x and y are independent and the value of the function $f(x, y)$ is dependent. In contrast, thermodynamics treats all variables equally and which variables are considered to be dependent and independent may change during data taking and analysis.

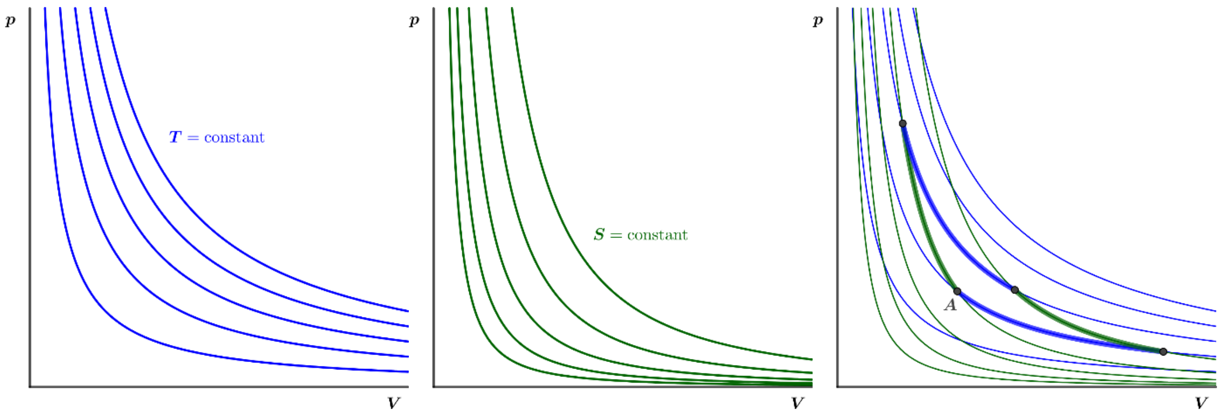

Figure 2: Contour plots of data from experiments on a piston. Fig 2a shows constant temperature isotherms, Fig 2b shows constant entropy adiabats, and the bold contour in Fig 2c shows a Carnot cycle.

What does not change is the number of independent variables. For a given experiment, the number of independent variables is equal to the number of ways of getting energy into/out of the system. In the piston experiment, this number is two: through heating and/or through doing mechanical work on the system. A scientist usually thinks of the variables that the experimenter controls as independent. Here, one would consider temperature (or entropy) to be the independent. Then, either pressure or volume can be chosen to be independent, but not both. Experimentally, it may be easiest to control the pressure, by adding or subtracting weights from the top of the piston and then to measure the resulting volume.

TYPES OF CONTOUR GRAPHS

This flexibility in interpreting which variables are independent and dependent has significant consequences for the interpretation of contour plots. In the conventional interpretation of a contour plot, such as a topographic map of a hill, the independent spatial variables x and y are plotted on the horizontal and vertical axes, respectively, and values of the dependent variable, height, are contours. In Figure 2, from the point of view of the experiment, the independent variables are plotted as contours and on the vertical axis, while the dependent variable, volume, is plotted on the horizontal axis!

Nevertheless, in thermodynamics, it is more common to plot p vs. V, as in Figure 2, because in the analysis, most often the scientist wants to calculate the work done on the system given by

$$W = -\int p \; dV,$$

interpreted in standard calculus language as "the area under the curve." Now we have switched our point of view, so that the volume is independent, the pressure is dependent, and the temperature is a parameter that specifies which run of the experiment is being considered.

DERIVATIVES FROM CONTOUR GRAPHS

Returning to Figure 2c, we might also want to determine the partial derivative $\frac{\partial p}{\partial V}$, the main contributor to the bulk modulus. The figure makes it immediately clear that one must ask, not only at what point, but also along which curve, should I calculate the derivative? Thermodynamics provides a generalization of Leibniz notation for these choices

$$\left(\frac{\partial p}{\partial V}\right)_T \text{ or } \left(\frac{\partial p}{\partial V}\right)_S$$

to indicate the curve with T held constant (and similarly for S held constant).

As an additional complication, in contexts where one does not have an algebraic expression for a function, e.g. discrete tables of data or graphs, finding a derivative (at a point) always involves determining small changes in both the numerator and the denominator variables and then calculating the appropriate ratio. Of course, a ratio of small changes only gives an approximation to the derivative. The limit process to find an exact value for the derivative is impossible. Just as in everyday speech, if you ask, “What is the temperature outside?” the answer “in the mid-20’s (Fahrenheit)” is sufficient to tell you that you need a coat. You wouldn’t bother to specify, “What is an approximation to the temperature outside?” In the same way, scientists will call this ratio “the derivative” so long as the shared understanding is that the approximation is good enough.

What remains is to decide which two points to use to find the ratio of small changes. The two points must lie along a curve for which the desired variable is being held constant—a clear indication that the considerations in the previous section are crucially important. Also, the two points must be close enough together that they lie in the regime where the function is changing linearly, to the degree of accuracy necessary for the application, but not so close that the difference between the values of the numerator (or denominator) variable cannot be sufficiently determined from the accuracy of the information. Here it is crucially important that the scientist have a clear understanding of the accuracy of the data, the accuracy with which the information can be read of the graph, and the size and spread of the fluctuations of the information.

PHYSICS EDUCATION RESEARCH AND CURRICULAR MATERIALS FROM THE PARADIGMS PROJECT

In the epistemological analysis above, we see that the interpretation of which variables are independent, dependent, or parameters in applied settings like thermodynamics is fluid (pun intended). The interpretation may change between the taking of data and its analysis. Furthermore, the calculation of a (partial) derivative depends on whether the given information is in the form of discrete data or an analytic formula. For more than 25 years, the Paradigms project at Oregon State University has been studying the epistemological differences amongst experts in different fields and the development of these disciplinary understandings in advanced undergraduate students, using a variety of interrelated theoretical perspectives contained within social constructivism. This research work has been intertwined with the development of curricular materials and hands-on manipulatives for thermodynamics and other middle-division physics courses.

A brief review of relevant research from the Paradigms Project can be found in the next section. Relevant curricular materials can be found on our website (Paradigms Team, 2015–2024a), and a short description of those materials that addresses derivatives can be found in Dray et al. (2019). A lovely, short classroom activity that asks students to confront many of the issues raised in this paper can be found in Paradigms Team (2015–2024b).

RESEARCH ABOUT STUDENT UNDERSTANDING OF DERIVATIVES FROM CONTOUR GRAPHS

Emigh and Manogue (2024) conducted semi-structured, think-aloud, problem-solving interviews with nine Paradigms students asking them to find the derivative at the indicated point A of a $p-V$ diagram, similar to Figure 2c, where the Carnot cycle changes from holding temperature constant to holding entropy constant. Thought of as a graph of a function of one variable, this is a point where the function is continuous, but the derivative is not. We were curious about what reasoning the students might use, from mathematics reasoning ("I can calculate the derivative from the left and the right, but they are different.") to physics reasoning ("Do you mean holding the temperature constant or the entropy?"). Interestingly, the thematic analysis showed that even when these interviewees demonstrated that they understood both math and physics concepts, they usually didn't relate them without prompting. Only one interviewee spontaneously realized that the two derivatives (one for the blue curve and one for the green curve) can be viewed as partial derivatives with the corresponding variables held constant. Sections V and VI of this reference give several detailed transcript examples of student reasoning. Two important insights of this research are: While these learners were initially orienting themselves to the graphs, they were more likely to attend to the labels on the horizontal and vertical axes than the labels on the contours. Interviewees did not use the subscript notation in generalized Leibniz notation for holding a variable constant until they attempted to manipulate some equations symbolically and did not appear to connect this notation to their other understanding of derivatives.

In a separate study, Bajracharya et al. (2019) conducted semi-structured, think-aloud, problem-solving interviews with eight Paradigms students. Interviewees were asked a more difficult prompt: to determine a particular partial derivative from data with some presented in a contour graph and other data presented numerically in a table. To solve this problem successfully, interviewees needed to identify which partial derivative could be found from the data as presented and calculate the correct ratios of small changes. Although this aspect of the problem was not the main focus of the thematic analysis of that paper, section V includes description of the problems interviewees had identifying which variables were present in the table of data and/or the contour graph and in using this information to find appropriate partial derivatives. These tasks are clearly challenging for middle-division students.

SUMMARY

Variables in thermodynamics like temperature and pressure do not have the same automatic identification as independent or dependent as spatial variables such as x and y do for scalar fields such as electrostatic potential in electromagnetism. This fluidity in the identification carries over to the interpretations of contour diagrams. We have provided some pointers to research from the Paradigms in Physics team and to related curricular materials that may be of use to researchers, curriculum developers, and teachers.

An observation from Emigh & Manogue (2024) states, “As instructors, we were especially encouraged to see that prompts from the interviewer shifted students’ attention dramatically. The prompts consisted of some variant of ‘Did you think about holding anything constant?’ and led most students both to solve the problem and to make sense of it—and they proceeded to use different language (e.g., ‘partial’ derivatives with some variable ‘held constant’) and different notation (e.g., subscripts) than before these prompts.” This observation suggests that small curricular changes may be very powerful.

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