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Collaborative Research: Research on the Learning and Teaching of Thermal Physics

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Final Report for Period: 07/2007 - 01/2008 **Submitted on:** 03/29/2008
Principal Investigator: Thompson, John R. **Award ID:** 0406764
Organization: University of Maine
Submitted By:

Title:
Collaborative Research: Research on the Learning and Teaching of Thermal Physics

Project Participants

Senior Personnel

Name: Thompson, John

Worked for more than 160 Hours: Yes

Contribution to Project:

PI on the project at the University of Maine. Coordinating research efforts in relevant courses, including research agenda (development and administration of questions to students in various courses as written questions or in individual student interviews, arranging for administration of written questions in courses in other departments at U. Maine and at other universities (Cal. St. U. - Fullerton, U. New Hampshire); assisting with and advising on data analysis and instructional materials development; scheduling and oversight of presentations at local, regional, and national meetings and conferences; working with colleagues on articles for publication (peer-reviewed conference proceedings to date; journal manuscripts will be prepared soon based on previous proceedings).
Support: (a) from grant - 1 month of summer salary each year of grant; (b) from department - academic year workload is 50% teaching, 50% research, and some startup funds for summer salary.

Name: Mountcastle, Donald

Worked for more than 160 Hours: Yes

Contribution to Project:

Instructor of courses in which majority of research took place ('Thermodynamics' and 'Statistical Mechanics'); assisted in development and analysis of questions designed to probe student understanding of specific concepts in thermal physics. Assisting with and advising on data analysis and instructional materials development.
Gave poster presentations on more than one occasion. Assisted with preparation of other oral and poster presentations for several local, regional, and national meetings.
Working with colleagues on articles for publication (peer-reviewed conference proceedings to date; journal manuscripts will be prepared soon based on previous proceedings).
Support: (a) from grant - 0.5 month of summer salary each year of grant; (b) from department - academic year workload is 50% teaching, 50% research.

Post-doc

Name: Christensen, Warren

Worked for more than 160 Hours: No

Contribution to Project:

Christensen is working on this project (since 8/1/2007) as a postdoctoral research associate, **supported by the University of Maine Center for Science and Mathematics Education Research**, and not this grant.
Christensen has contributed to the project in several ways. He worked as a graduate student with our collaborator David Meltzer (PHY-0406724, -0604703), and brings his experience with this work, primarily at the introductory level, to our work at the advanced level. He has helped with data analysis and curriculum development, providing input and insight to many topics.

Graduate Student

Name: Bucy, Brandon

Worked for more than 160 Hours: Yes

Contribution to Project:

As the senior graduate student (and only doctoral student) on this project, Brandon has done the majority of the work 'in the trenches.' Assisted in development of and conducted bulk of analysis of questions designed to probe student understanding of specific concepts in thermal physics. Conducted individual interviews of students to probe understanding more deeply. Writing instructional materials to address student difficulties found in written and oral responses to above questions.

Has given oral and poster presentations on findings at several local, regional, and national conferences. Working with colleagues on articles for publication (peer-reviewed conference proceedings to date; journal manuscripts will be prepared soon based on previous proceedings).

Support: (a) from grant - 50% research assistantship during academic year for years 1 and 2, and 1/3 assistantship Year 3 of grant, and full research assistantship in June 06; (b) from graduate school - Summer Graduate Research Fellowship, 2005.

Brandon successfully defended his dissertation in July 2007. Dissertation work focused on (1) student understanding of entropy in physics and other science and engineering courses, at UMaine and at collaborating institutions, and (2) student understanding of mixed second-order partial derivatives in the context of material properties and the Maxwell relations. For (2), a set of curricular materials was developed to improve students' connections between the mathematics and the physics. Preliminary data show increased performance later in the course on questions involving partial derivatives.

Name: Pollock, Evan

Worked for more than 160 Hours: Yes

Contribution to Project:

Evan is a graduate student (M.S. candidate) who started on the project in the summer of 2006. He is working on student understanding of P-V diagrams, and how students use them to solve problems in thermodynamics, both in a physical and a mathematical sense. He has analyzed previously collected as well as new data, and expanded the scope of the analysis. He has assisted with the preparation and administration of research questions, and with archiving of data. He has analyzed data relevant to his thesis project as well as assisted in analysis and interpretation of additional data.

His work was supported by a 1/3 research assistantship during the 06-07 academic year and a 1/2 research assistantship in Summer 2007; remaining support was from teaching assistantships. Most recently he has been partially supported by Grant #REC-0633951, which is looking at student thinking about mathematics in physics contexts, so it is completely commensurate with his work.

Undergraduate Student

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Organizational Partners

University of Washington

Partner in Collaborative Research Grant. David Meltzer moved from Iowa State University to the University of Washington. We have had discussions with our collaborators, David E. Meltzer and Warren Christensen (who is currently a Postdoctoral Research Associate at the U. Maine Center for Science and Mathematics Education Research) on research tasks; exchanged instruments and administered questions developed by our collaborators to our students (and vice-versa); shared and compared data; discussed and collaborated on instructional materials development.

Meltzer and Christensen used one set of our questions to develop curricular materials for an introductory physics course. Later, we revised those materials, with Christensen's help, to use them in an upper-level thermodynamics course.

We have given joint and/or connected presentations at national meetings, and will prepare and submit a joint manuscript in the next six months.

Other Collaborators or Contacts

We have administered written questions in other classes, both at U. Maine and at other institutions. At U. Maine, we administered questions in CHY 471 (Physical Chemistry I) with the permission of the instructor, Dr. Jay Rasaiah in Fall 2005, and in CHE 385 (Chemical Engineering Thermodynamics I) with the permission of the instructor, Dr. John Hwalek, to investigate the different approaches to thermal physics in different disciplines. We obtained data from two semesters of CHE385 - one pre-instruction (Spring 2006) and one post-instruction (Spring 2007), which was very helpful for investigating student learning in the course. We are planning on obtaining more data in the Spring 2008 semester from CHE385.

We also administered questions at other institutions in the Spring 2006 semester: in PHYS 508 (Thermodynamics and Statistical Mechanics) at the U. of New Hampshire, taught by Dr. Bill Hersman, with data collection assisted by Dr. Dawn C. Meredith, and in PHY 310 (Thermodynamics, Kinetic Theory, and Statistical Physics) at California St. U. - Fullerton, with the permission and input of the instructor, Dr. Michael E. Loverude.

We especially look forward to more collaboration with Dr. Loverude, who has expertise in Physics Education Research on thermodynamics at the introductory level, and has been himself conducting research on student learning in his PHY 310 course for several years.

Finally, in 2006 we had the opportunity to administer some of our questions to High School AP Chemistry and Physics Teachers participating in a professional development workshop on thermodynamics, with the permission of the facilitator, Mr. Michael Schaab.

In 2005-2006, we distributed questions and materials to Seattle Pacific University (H. Close). In 2006-2007, we distributed questions and materials to the following institutions: Southern Illinois University-Edwardsville, R. Lindell; Pacific University (Forest Grove, OR), S. Hall. In 2007-2008 we have added Trininjan Datta, from Augusta State University (GA) to our list of pilot sites. Dr. Datta has administered questions both pre- and post-instruction.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

Findings: (See PDF version submitted by PI at the end of the report)

Training and Development:

This project has provided a context for professional development of the PI, the Senior Personnel, and the Graduate Research Assistants. The PI has brought his experience in empirical PER û identifying student difficulties, development of curriculum, and assessment of the effectiveness of instruction û to the arena of upper-division thermal physics. He has learned a great deal from the Senior Personnel about teaching material of this nature and of the subtleties in the material, both physically and mathematically.

The Senior Personnel, a senior faculty member with long-standing interests and self-motivated experience in gauging the impact of teaching on student understanding, has been exposed through this project to the research methodologies and analysis techniques in PER. He has made significant contributions to the project, especially in terms of identifying specific content areas that he recognizes as particularly difficult for students. Several questions developed by the project team have been derived or taken wholesale from questions he has devised, especially in the areas of material properties and partial derivatives, equations of state and variables, and probability and statistical uncertainty.

He is currently lading the research effort for one of the topical research projects, on probability and uncertainty.

The doctoral student who worked on the project has done the bulk of question development, data analysis, and instructional materials development. He has learned many of the typical research methodologies used in empirical PER, including individual student interview techniques and different ways to interpret student responses in different contexts. He has produced high-quality, accessible presentations, both oral and written.

He defended his dissertation in August 2007. He has been hired as a postdoctoral reserach associate on a different grant, and is excellently prepared to supervise research projects; he will be quite successful as a faculty member.

The master's student has learned a great deal about both content and pedagogy, as well as research methods in PER. His training has included the conduct of individual student interviews. Through the preparation and delivery of oral and poster presentations, and from the preparation of a manuscript under the PI's supervision, his written and oral communication skills are improving significantly.

He will defend his M.S. thesis in the summer of 2008.

Additional graduate students - currently in their first year - have been recruited to work on this project as of the beginning of the calendar year. They saw this project as very interesting and cutting edge. One is particularly interested in the curriculum development and assessment pieces, and others are interested in the investigations of student knowledge at the math-physics interface.

Outreach Activities:

None on this topic. In outreach activities in which we participate, we do mention our research findings as they may be relevant. The audience most often is high school physics teachers. We anticipate running faculty workshops for any curricular materials developed during the next phase of the project, once a sufficient number of tutorials are developed. We are currently developing several 'tutorials' based on explicit research results as well as the appropriate pedagogy for gaining a deeper conceptual understanding of a topic.

Journal Publications

Brandon R. Bucy, John R. Thompson, and Donald B. Mountcastle, "What Is Entropy? Advanced Undergraduate Performance Comparing Ideal Gas Processes", 2005 Physics Education Research Conference, AIP Conference Proceedings, p. 81, vol. 818, (2006). Published,

John R. Thompson, Brandon R. Bucy, and Donald B. Mountcastle, "Assessing Student Understanding of Partial Derivatives in Thermodynamics", 2005 Physics Education Research Conference, AIP Conference Proceedings, p. 77, vol. 818, (2006). Published,

Bucy, B.R., Thompson, J.R., and Mountcastle, D.B., "Student (Mis)application of Partial Differentiation to Material Properties", 2006 Physics Education Research Conference (AIP Conference Proceedings), p. 157, vol. 883, (2007). Published,

E.B. Pollock, J.R. Thompson, and D.B. Mountcastle, "Student understanding of the physics and mathematics of process variables in P-V diagrams", 2007 Physics Education Research Conference (AIP Conference Proceedings), p. 168, vol. 951, (2007). Published,

D.B. Mountcastle, B.R. Bucy, and J.R. Thompson, "Student estimates of probability and uncertainty in advanced laboratory and statistical physics courses", 2007 Physics Education Research Conference (AIP Conference Proceedings), p. 152, vol. 951, (2007). Published,

Books or Other One-time Publications

Brandon R. Bucy, "Investigations of Student Understanding of Entropy and of Mixed Second-Order Partial Derivatives in Upper-Level Thermodynamics", (2007). Thesis, Published
Bibliography: Ph.D. dissertation (Physics), University of Maine

Web/Internet Site

Other Specific Products

Product Type:

Teaching aids

Product Description:

Small-group, guided-inquiry instructional materials - a tutorial titled "Partial Derivatives and Material Properties" - designed to help students recognize the physical significance of mixed partial derivatives and the graphical interpretation of partial deriviatives in general.

(Tutorial is attached at end of "Findings" file.)

Sharing Information:

After pilot-testing this tutorial at U. Maine, we will send it to instructors willing to use it in their classes.

Product Type:

Teaching aids

Product Description:

Small-group, guided-inquiry instructional materials - a tutorial titled "Entropy Changes in Ideal Gas Processes" - designed to help students recognize the various features of entropy and its relation to the second law of thermodynamics inthe context of ideal gas processes (isothermal expansion, free expansion).

(Tutorial is attached at end of "Findings" file.)

Sharing Information:

We will send to any interested parties once pilot-testing and revisions at our institution are complete.

Product Type:

Teaching aids

Product Description:

Small-group, guided-inquiry instructional materials - a tutorial titled "Multiplicity and the Density of States" - designed to help students recognize the relationship between multiplicity and the density of states, and to begin to use that relationship to determine other properties, such as entropy. This is seen as the first in a sequence of tutorials using the density of states as a central concept.

(Tutorial, as well as a guide for instructors intending to use it, are attached at end of "Findings" file.)

Sharing Information:

Once the tutorial is sufficiently tested at our institution, we will disseminate it for secondary implementation.

Contributions

Contributions within Discipline:

This project is identifying areas in the teaching and learning of thermal physics at the advanced undergraduate level in which students have specific conceptual difficulties. We are cataloging, in a sense, the state of knowledge of students in these courses before, during, and after instruction.

One major finding that we are pursuing is the relationship between mathematics and physics at this level. Our results strongly suggest that a functional understanding of how relevant mathematical concepts apply to the physical situations presented in these courses is not an outcome of prerequisite courses in either mathematics or physics. Some aspects of this material are improved in the relevant courses, but still not to a satisfactory level for instructors.

This project is raising the awareness of the need to provide explicit instruction (or at least context-specific review) of mathematical concepts rather than to assume facility with applications, when teaching at the upper division.

Recent results from questions administered at the end of third-semester calculus courses further underscore the importance of this research and the exploration of the use of mathematics by students in physics courses.

Furthermore, we are speaking to a debate that has taken place in physics education for years: the tension between a macroscopic, phenomenological viewpoint and a statistical, particulate view to teach physics concepts, most notably thermodynamics. Our work with entropy indicates that both views need to be understood and utilized appropriately by students for a complete understanding of entropy in the context of thermodynamic processes. This finding should generate considerable discussion.

Contributions to Other Disciplines:

Our results from Chemistry and Chemical Engineering courses has provided evidence for the effectiveness of different pedagogical approaches with respect to entropy, and we plan to publish and present these findings in the near future.

Our work will hopefully improve dialog between our disciplines in teaching similar material.

Our results with application of mathematics may lead to discussions of the need for more examples of applications in relevant mathematics courses (e.g., the physical meaning of partial derivatives, and the connection between Clairaut's Theorem and the Maxwell relations, in Calculus III).

We have begun to explore even more basic calculus concepts (integrals and derivatives) in our work, and will be contributing to the body of research on this topic. We find that even after instruction in Calculus III, students have difficulties ranking derivatives of graphed functions, or comparing the magnitudes of integrals of different functions with the same endpoints. Some of this has been reported for introductory courses, but not among advanced students in physics or mathematics courses.

Contributions to Human Resource Development:

This project has served as the venue for training of one doctoral student and one master's student. The doctoral student is continuing in research on student learning with a postdoctoral appointment, with eventual plans for a faculty position. The master's student has plans to obtain a doctorate in physics doing physics education research. Both students have gained significant experience with research methodologies and 'reform' pedagogical methods. By the end of this project, additional doctoral students have expressed interest, and two postdoctoral research associates have contributed to the work (both of whom were graduate students on this project).

Results of this project are informing the development of instructional materials to improve student learning in thermodynamics, in making connections between physics and mathematics, and in appreciating common concepts across disciplinary boundaries.

Contributions to Resources for Research and Education:

This work is groundbreaking in more than one way. By employing methodologies proven at the introductory level to students at the advanced level, and in other disciplines, we are demonstrating the effectiveness of physics education research methodologies beyond introductory physics, and in the separation of conceptual difficulties as mathematical or physical in nature. The work related to the math-physics interface in this project has attracted attention from many researchers and educators.

Our work has inspired similar research in chemical education research, with a CCLI proposal submitted in January 2008. John Thompson was asked to be a consultant on that project due to his work on this project.

The continued development of instructional materials based on the research will also help both research on student learning and the learning itself.

Contributions Beyond Science and Engineering:

Conference Proceedings

Categories for which nothing is reported:

Any Web/Internet Site

Contributions: To Any Beyond Science and Engineering

Any Conference

The majority of our findings relate to the identification of specific conceptual and mathematical difficulties among students when learning this material using traditional thermal physics textbooks and teaching methods. Details are given for several topics below.

Student understanding of entropy across disciplines

As mentioned in our previous report, our investigations into student understanding of entropy and the Second Law consisted of an analysis of written student responses to a researcher-designed set of free-response diagnostic questions. (See supplemental documents.) Data gathered in clinical interviews with individual students were employed to illustrate and extend results gathered from written student responses. The question sets provided students with several ideal gas processes, and asked students to determine and compare the entropy changes of the processes. We administered the question sets to students from six distinct populations, including students enrolled in classical thermodynamics, statistical mechanics, thermal physics, physical chemistry, and chemical engineering courses, as well as a sample of physics graduate students. Data was gathered both before and after instruction in several samples. For this grant year, we obtained another round of data from our classical thermodynamics course (both pre- and post-instruction), and from the chemical engineering thermodynamics course (post-instruction; previous data were obtained pre-instruction) to use in the analysis.

During this year the entropy data from the many classes were deeply analyzed, and results between the different disciplines compared. Several noteworthy features of student reasoning have been identified. These features include the ways in which students think about entropy prior to instruction as well as specific difficulties and other interesting aspects of student reasoning that are evident after instruction.

Prior to instruction, several students incorrectly related entropy to concepts previously covered during the course. These students related entropy to temperature (not temperature multiplicity), work done, and to the internal energy of the system under consideration. Many of these incorrect relationships were not present in the post-instruction samples, suggesting they had been refined into correct relationships between entropy and related concepts. At the same time, some of these difficulties were persistent.

Many students from the pre-instruction samples also expressed the idea that entropy represents some form of disorder, and that entropy increases as this disorder increases. Students rarely elaborated on the basic disorder idea, sometimes referring to it as “randomness,” “chaos,” or a “breakdown of order.” We have documented in several student samples the successful refinement of this basic concept of disorder into a more sophisticated approach to entropy from a statistical standpoint. Students connect disorder with volume, or spatial multiplicity concepts in their responses to the post-test. It appears that students’ basic entropy-as-disorder beliefs naturally resonate with the concept of the spatial arrangement of the constituent particles of a system. And yet, the refinement of disorder into a complete statistical approach to entropy remains incomplete among the student samples studied. While disorder is linked to volume multiplicity, a corresponding link is not made to temperature multiplicity. Furthermore, students often fail to fully explain the statistical underpinnings of the relationship between volume and entropy. Future avenues of research involve a deeper exploration of student statistical reasoning, including the statistical basis of volume multiplicity, and the statistical basis of temperature multiplicity.

Students consistently underutilized the state function property of entropy. Students fell into two groups with regard to state function reasoning, either explicitly regarding entropy as a state function, or implicitly comparing entropy changes by looking at other, related state functions. The implicit application of state function reasoning was invariably tied to students' use of multiplicity-based reasoning (ranking by volume, in particular), while the students who explicitly applied state function properties to entropy did not refer to multiplicity arguments in their answers; they used thermodynamic reasoning instead.

We have identified a number of specific applications and misapplications of the Second Law in student reasoning. The tendency to incorrectly apply the Second Law to the system, or to the surroundings, is notable among the misapplications. (Students employing this tendency treat the system (or surroundings) entropy change as the entropy change of interest, rather than the universe entropy change). Also notable is a tendency among students to reason from a conservation principle of universal entropy. Students tend to employ the Second Law more faithfully after instruction, although the Second Law is rarely used as a check for responses determined via other methods. A related aspect of student reasoning among chemistry students seems to be the confusion between the two criteria for spontaneity represented by the Second Law and by changes in the Gibbs free energy of a system. Several of these students appeared to ascribe aspects of Gibbs free energy to entropy in their responses to the diagnostic questions, while others were unaware of the constraints imposed upon the Gibbs criterion (isothermal and isobaric processes only). This result is in accord with those of chemical education researchers.

On a larger grain-size note, students from various populations tended to reason about entropy either via a thermodynamic approach – reasoning about heat transfer or using the thermodynamic definition of entropy – or via a statistical approach – reasoning about the volume occupied in terms of spatial multiplicity. Temperature considerations were lacking in all student samples, suggesting a general conceptual disconnect between temperature and the statistical approach. Both approaches present students with a unique set of benefits as well as challenges. Elaboration: Students who combined these approaches performed the highest on the diagnostic question sets. Students preferred the statistical definition of entropy in reasoning tasks, particularly the concept of spatial multiplicity. While expected, the results are nonetheless interesting due to the fact that many of these students were enrolled in a purely classical thermodynamics course, where most instruction and all homework questions dealt exclusively with the thermodynamic definition only. Although students readily identified with the statistical interpretation of entropy, our results suggest that their understanding remains incomplete, confined mainly to the spatial aspect of multiplicity and not taking into account the momentum/temperature aspect of multiplicity.

In an attempt to address some of the student difficulties with the state function concept of entropy described above, in Fall 2007 we revised a curricular worksheet designed by collaborators Warren Christensen and David Meltzer to allow for its use in an upper-level thermodynamics course. The revised tutorial is included at the end of this document. The tutorial, ***Entropy Changes in Ideal Gas Processes***, begins by introducing students to the thermodynamic definition of entropy, which is applicable only for calculating *reversible* entropy changes. Two processes are then presented, one a reversible isothermal expansion, and one an irreversible free expansion, to lead students to the idea that *irreversible* entropy changes can be calculated as well by exploiting the state function aspect of entropy: all one must do is find a reversible process that starts and ends at the same states as the irreversible one does.

In concert with the revised tutorial, a post-test question was designed that presents students with an irreversible ideal gas process (a throttling process; see attached file at the end of this document). In order to calculate the entropy change for this process, students needed to identify a reversible process that begins and ends at the same state as the throttling process, calculate the entropy change for that reversible process, then exploit the state function property of entropy to argue that the irreversible entropy change must be the same value. The tutorial was implemented in Fall 2007; video data was gathered of two student groups working through the tutorial.

Based on preliminary results gathered in the Fall 2007 semester of the *Physical Thermodynamics* course, it appears that the tutorial was a qualified success. Three of the five students who completed the post-test correctly calculated the entropy change for the throttling process. However, only *one* of these students explicitly used the method presented in the tutorial, while at least three students used a *TdS* equation provided on an attached equation sheet to calculate the entropy change (only one arriving at the correct answer with this approach). The remaining correct student implicitly used state function reasoning, although it is not evident from the student's reasoning that the student was aware of this fact.

Widespread student difficulties with applications of mathematics prerequisites

A major component of our research involves how students view, use, and understand the underlying mathematical concepts in the context of thermodynamics. We have identified several difficulties that are mathematical in nature; at least one of these was previously identified as a physics conceptual difficulty, and our results show that some of the students exhibiting this difficulty may have mathematical conceptual issues rather than, or in addition to, any problems with the physics concepts.

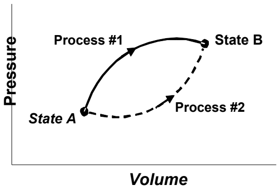
The general theme of this work is probing mathematical meaning and physical significance in physics. We explain results of analysis that occurred primarily during the past project year.

- *Integrals; path dependent or not, anti-derivatives, Riemann sums*

Students were asked several questions regarding first law quantities along with similar mathematical questions devoid of all physical context. We compared student responses to physics questions involving interpretation of ideal gas processes on P-V diagrams and analogous mathematical qualitative questions about the signs and comparisons of magnitudes of various integrals. Overall results coupled with individual student performance on the paired questions shows evidence of isolated understanding of the physics and/or the math, although some difficulties are addressed by instruction.

Meltzer (*Am. J. Phys*. **72**, 1432-1446 (2004)) developed a set of questions probing student understanding of the First Law and related quantities based on processes shown on a *P-V* diagram. These are shown below.

This Pressure-Volume *(P-V)* diagram represents a system consisting of a fixed amount of ideal gas that undergoes two ***different*** processes in going from state A to state B:



[In these questions, ***W*** represents the work done ***by*** the system during a process; ***Q*** represents the heat transfer ***to*** the system during a process.]

P1. Is *W* for Process #1 ***greater than, less than***, or ***equal to*** that for Process #2? Explain.

P2. Which would produce the largest change in total energy (kinetic plus potential) of all the atoms in the system: ***Process #1, Process #2***, or ***both produce the same change***?

In addition to replicating Meltzer's experiment in our upper-level thermodynamics course, we wanted to know if some of the conceptual difficulties might originate in the mathematics. We asked about the work done by, heat transferred to, and the internal energy changes in an ideal gas sample during two different process that each started at the same state and ended at the same state. We also designed questions that are analogous to Meltzer's questions, but purely mathematical in nature – all physics is removed from the setting. For the math question analogous to the work comparison question, we asked students to compare the magnitudes of the integrals of two functions over regions that that both started at the same point and ended at the same point, but were clearly different functions.

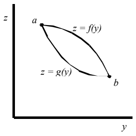
While some students gave correct answers, many of the students said that the works were equal. The physics explanation inferred by the reasoning used for this incorrect response is that students are treating work as if it were a state function, independent of path. This is a reasonable conclusion, until one examines the results of the analogous math question. Of the "equal works" students, more than half also gave incorrect integral comparisons, showing that some of the difficulties assumed to have their origins in the physics were actually (or additionally) mathematical in nature.

This year in the project, we asked the physics questions *after* instruction on the first law and more practice with *P-V* diagrams. Not too surprisingly, instruction leads to better results (although our data are from one class of 6 students): 5 of 6 students correctly compared the works, and none of the students said that the works were equal.

Two functions have been graphed on the *z-y* graph shown at right, and are labeled *f(y)* and *g(y)*. Both functions start at point *a* and end at point *b*.

Consider the integrals

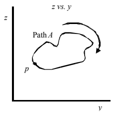
$$I_1 \equiv \int_a^b f(y)\,dy \quad \text{and} \quad I_2 \equiv \int_a^b g(y)dy$$



Is the absolute value of integral I_1 ***greater than***, ***less than or equal to*** the absolute value of integral I_2, or is there ***not enough information to decide***? Please explain.

Math question analogous to work comparison (P1).

H is a function of the independent variables *z* and *y*; i.e., *H* = *H(z, y)*. A path has been traced out on the *z-y* graph at the right, and has been labeled Path *A*.



Consider the closed path integral

$$I_2 \equiv \oint_{A\,,clockwise} dH$$

where the path starts at point *p* and proceeds clockwise around Path *A*.

Is the integral I_2 ***positive*, *negative*, *zero***, or is there ***not enough information to decide***? Explain.

Math question analogous to internal energy comparison (P2).

A second question in this set has been examined for its implications about student understanding of the mathematical significance of the state function. 20 of 21 students correctly stated that the internal energy changes were equal between the two processes, often using state function reasoning explicitly or indirectly (e.g., path independence). The analogous math question however, was much more difficult for students. Recognition that the integral of *dU* yields an antiderivative on a *P-V* diagram of a closed ideal gas system allows for the parallel question to be asked: consider a two-dimensional function *H(z,y))*, and integrate *dH* over a closed loop. By labeling *(H(z,y))* as a *function* we have required it to be single-valued over the *z,y* domain. When evaluating a closed cyclic path integral, the only value of interest is the value on the path at the location of interest (point P). The integral of dH becomes the antiderivative *(H(z,y)),* according to the Fundamental Theorem of Calculus. When the antiderivative is evaluated at *P*, the common start and end point, the result of the integration is zero.

Only about half of the students—10 out of 21—were able to provide correct responses on this math question. We believe that a contributing factor to the high success rate on the physics question is that state function reasoning, incorrectly applied to work in the earlier question, is correct for *H(z,y)*. Our results show that a basic understanding of the physics concept (e.g., path independence of changes in state variables) does not imply a basic understanding of the analogous mathematics or functions. It may be that instruction in properties of state functions results in purely algorithmic understanding and may be highly context specific. These two aspects share a common thread in that students apparently fail to recognize the mathematical information describing the physical process(es). This thread is shared by our results mentioned below about partial derivatives.

Associated with the above mentioned problems with exact and inexact differentials is a related mathematics difficulty, namely the lack of distinction between path-dependent and path-independent integrals, specifically in the context of *P-V* diagrams and determinations of work, heat and internal energy changes. This result has been interpreted as a failure to adequately distinguish between the related concepts of the Riemann sum and the antiderivative. Other researchers have hypothesized that student difficulties with path dependent and path independent integrals stems from a lack of understanding of the physical phenomenon in question, however our results suggest that an unfamiliarity with the underlying math may be equally or even more important.

This research and analysis is ongoing, and has been conducted primarily by M.S. candidate Evan Pollock, with initial investigations by Brandon Bucy (Ph.D. 2007).

- *Probability, variance and uncertainty as functions of N*

Macrostates, microstates, multiplicity, probability, fluctuations, uncertainty, entropy, equilibrium, and reversibility are all necessary concepts for mastering thermal physics, essential in varying degrees in all of the thermal physics courses in our research program. This is especially so in statistical mechanics, where we are conducting the majority of our research on the teaching and learning of statistical concepts. Typical statistical physics textbooks introduce entropy (S) and multiplicity (ω) [$\mathsf{S} = \mathsf{k}\ln(\omega)$; k is Boltzmann's constant] by using coin flips and/or other such binary process outcomes, repeated N times. A large majority of our statistical mechanics students has previously completed at least one Mathematics Department statistics course, and an even larger majority has completed one of our laboratory courses that included an extended group project using the students' dart scores on a one-dimensional target. That project required graphing the dart score data set, analyzing and comparing with a Gaussian distribution, as the number of reported scores (N) increased from ~ 20 to > 200; questions asked for predictions, as well as quantitative values of mean, standard deviation, standard deviation of the mean, and several questions with explanation about the distribution, especially the dependence on N of various parameters.

Prior to instruction, we collected several iterations of our students' predictions for the number of heads *with uncertainties* as N increases from 4 to 1000 to N_A (6×10^{23}), as well as measurement uncertainty of a continuum (amount of rainfall) as a function of the number of measurements. Our students reliably give correct answers for the expected $N/2$ heads out of N coin tosses, whether 1 coin is flipped N times, or N coins are randomly mixed and shaken together. They also reliably predict the uncertainty in measured rainfall should *decrease* with an increasing number of spatially distributed measurements averaged together. However, only half of the students in four successive classes (2005-2008) predicted a decreasing *relative uncertainty* in the number of expected heads, as the coin flip N increases. (We also have related data from the laboratory darts exercise showing widespread conceptual confusion between the standard deviation of a distribution with the standard deviation of the mean.) Most surprisingly, several (20%) in fact gave answers of $N/2 \pm N/2$ heads (i.e., the *entire range* of N flips), even for $N = 1000$ and N_A coin flips. We interpret this as a difficulty in the conceptual transition from the discrete to the continuum as N increases from 4 to $\sim 10^{23}$.

Statistical physics textbooks typically introduce small numbers of binary events where microstates, macrostates, multiplicity and probability can be easily counted and calculated, then quickly extrapolate to large numbers and argue that with increasingly overwhelming probability the most likely outcome is the $N/2$ macrostate. This semester, after instruction on these topics including the binomial coefficient [Baierlein, Chapter 2; and Carter, Chapter 12], a new question was included on the following assigned student homework, asking students to first *predict with explanation* the change in multiplicity *and* probability (increase, decrease, or same) of the most likely outcome for finding six distinguishable balls distributed in two bowls with the textbook similar example of four balls into two bowls. They then made the calculations, plotted histograms of all macrostates, and explained the outcomes with reference to their predictions. Half of our students predicted (after instruction) the $N/2$ symmetric macrostate would have both increased multiplicity and probability, while the other half predicted an increased multiplicity but with a *decreased* probability (correct) for the $N/2$ symmetric macrostate. In fact, using the binomial coefficient along with the 2^N total number of microstates, one can indeed show a higher multiplicity (20) for $N/2$ of 3 + 3 balls than the corresponding most probable macrostate multiplicity (6) of $N/2$ for 2 + 2 balls. However, the total number of possible microstates (2^N) increases even faster with N, giving a *reduced probability* of 20/64 for 6 balls compared to 6/16 for 4 balls. Standard textbook treatments usually emphasize the increased multiplicity and neglect the actual reduced probability with "overwhelmingly most likely" arguments. As a more dramatic example, the (exactly-) 500-heads outcome macrostate for 1000 coin flips has an actual probability of only 2.5% $[1000!/(500!)^2(2^{1000})]$. Clearly, after instruction using textbook presentations along with the binomial coefficient, many of our students still confuse the related concepts of *multiplicity* with macrostate *probability*. We are currently developing a tutorial exercise to help students clear up this confusion, and thus discover that the binary outcome expectation value clearly <u>must</u>, with increasing N, approach a relatively narrow collection of closely adjacent macrostates (not just one), centered at $X = N/2$, <u>with fluctuations</u> of $\pm\ \delta X$. Fluency in traversing the abstract range from the discrete to the continuum is a difficult conceptual challenge, but vitally important in all areas of physics, currently gaining even more importance along with the emerging variety of research and development in nanoscience.

This research and analysis is ongoing, and is being conducted primarily by Senior Personnel Donald Mountcastle. We have benefited greatly from discussions with Michael Loverude at California State University – Fullerton, who is conducting similar research and asking questions that are similar and complementary to ours.

- *Multivariable functions, partial derivatives, mixed second-order partial derivatives*

A number of thermal physics textbooks use a standard approach to the teaching of certain topics. Among these is the concept of a state function as a function whose integral is independent of path (or thermodynamic process). Textbooks provide several examples and sometimes even a mathematical appendix designed to teach students the distinction between exact and inexact differentials. In spite of explicit time and effort in the classroom, students often apply state function reasoning to inexact differentials as well as exact ones, and fail to notice the distinction made by the textbook authors.

Foremost in our math-physics research to date has been analysis of student understanding of partial derivatives, especially mixed second partial derivatives, in thermodynamics. We have asked several written questions and conducted interviews that probe student conceptual understanding of the physics, the prerequisite or underlying mathematics, and the connection between these ideas. The main question focused on here is known as the β–κ question, asking about a comparison of partial derivatives of the isothermal compressibility and the (isobaric) thermal expansivity. (See figure below.)

In general, students were able to discuss the mathematical distinction between a partial and a full derivative. Most students were able to translate the mathematical formula of a partial derivative into a verbal description of the process, and either explicitly mentioned or implied that other variables need to be held constant when dealing with partial derivatives, even if they did not consistently acknowledge this in their responses. Several students correctly answered the β–κ question, appealing to "the equality of mixed second partials." They were also able to perform the calculus necessary to solve a problem, albeit not without errors. Finally, most students were able to successfully derive the Maxwell relations from a given set of thermodynamic potentials.

(a) Show that in general $\left(\frac{\partial\beta}{\partial P}\right)_T + \left(\frac{\partial\kappa}{\partial T}\right)_P = 0.$

(b) With the usual definitions of isothermal compressibility *(κ)* and thermal expansivity *(β)*, for any substance where both are continuous, show how these two derivatives are related:

$$\left(\frac{\partial\kappa}{\partial T}\right)_P \quad \text{and} \quad \left(\frac{\partial\beta}{\partial P}\right)_T .$$

"*β*-*κ* question" asked to students on (a) homework and (b) a midterm examination. Based on a homework problem from the text.

A major difficulty documented in our work was the tendency among students to equate the mixed second partial derivatives of a state function to zero. Some students also treated differential expressions algebraically. Additionally, many students were unable to take a description of a physical process and produce a partial derivative that represented that process mathematically, even after instruction. Finally, many students had difficulty recognizing when a physical situation calls for the use of a Maxwell relation, and even fewer were able to select the appropriate Maxwell relation needed to solve a certain problem.

All of the successes delineated above have a common feature: a largely algorithmic, rather than conceptual, understanding. For example, construction of a verbal description of a partial derivative requires merely inserting the relevant physical variables in place of the mathematical symbols. In addition, the assertion that the mixed second partials of a state function are equal seems simply the application of a 'remembered result' from a mathematics class. The general inability of students from the 2006 semester to prove this result via application of the definition of a derivative supports this conclusion. Finally, with regard to the Maxwell relations, the existence of several mnemonics for generation of these relations attests to the algorithmic nature of this procedure.

In order to address some of the difficulties we observed and documented, we developed a set of instructional materials to guide students to the correct understanding and to make appropriate connections between the physics and the mathematics of partial derivatives, using a graphical interpretation of these quantities as the bridge. (These materials are included at the end of this document.) Specifically, we wished to replace algorithmic manipulations and applications of remembered formulae with the thoughtful *evaluation* of mathematical results in terms of graphical and physical interpretations. In addition, we tried to strongly encourage both the *interpretation* and the *mapping* steps, the steps that connect mathematics and physics.

The tutorial was implemented in the Fall 2006 and Fall 2007 semesters of *Physical Thermodynamics*. Field notes were taken during the first implementation and video data was gathered from two student groups during the second implementation. Based on these implementations, the tutorial was revised to address some minor sticking points encountered by the students.

Based on the preliminary results from two semesters of tutorial intervention, it appears that the tutorial was somewhat successful at replacing algorithmic knowledge with conceptual knowledge. Students performed better on both the β–κ questions and on later Maxwell relation questions than their counterparts had in previous semesters.

This research is ongoing, and has been primarily conducted by Ph.D. candidate Brandon Bucy. We have benefited from discussions with collaborators David Meltzer and Warren Christensen.

Overall, we plan to continue to examine student connections between mathematics and physics, in thermodynamics, but also in other contexts where it is reasonable.

As part of this plan, in Fall 2007 we developed a six-question math diagnostic quiz, which we administered to 5 sections of UMaine's undergraduate Calculus III course, taught by the mathematics department. The diagnostic quiz contains several questions asked in our thermal physics courses, including the integral questions and partial derivative questions described above, as well as several other questions dealing with the complementary concept of differentiation. (The calculus diagnostic quiz is included at the end of this document.) Importantly, the questions were asked in a completely mathematical context, without any reference to physical situations. Drafts were provided to the math faculty involved, and none of these instructors identified any of the questions as being inappropriate for their students (one question required minor revision to a mathematical expression to make the terminology consistent with that used in the course). Approximately 100 students answered at least one part of the diagnostic quiz.

Much of the data gathered is remarkably consistent with that observed in our thermal physics courses. On the Calculus I integral question, about 60% of students correctly identified the integrals as positive, while only 47% of students correctly determined that I_1 was greater than I_2. 28% of students stated that the integrals would be identical, using some form of path-independent reasoning. On the loop integral question, only 34% identified the loop integral of dH as being equal to zero. A unique response from calculus students (between 24% and 44% gave this response) was "negative," according to the reasoning that "the path is clockwise." This is a convention used in mathematics to evaluate *path* integrals, not regular loop integrals.

On the math-only version of the β–κ question, 22% of calculus students correctly equated the mixed second-order partial derivatives, while double that (40%) stated these partial derivatives identically equaled zero. Only a single student provided a completely correct response, with 98% of students answering incorrectly or employing calculus errors (incorrect product/chain rule usage, etc.). These results are particularly interesting, and quite remarkable, as they demonstrate that the errors observed in our thermodynamics courses are *not* the result of the different notation used in physics to characterize partial derivatives, but rather result from difficulties with the underlying mathematics, or difficulties in bridging physical intuition and mathematical formalism.

Additional questions were asked about the nature of the derivative as the slope of a tangent line. When asked explicitly about derivatives, 70% of students were able to determine the sign of a function's derivative at a certain point, and only 48% could correctly rank these derivatives. When asked specifically about ranking the slope of a certain function at several given points, performance was somewhat better at 80%, although this percentage is rather lower than most physics instructors might wish for such a simple task.

Finally, students were asked to differentiate a simple function composed of two different functions of a single variable. One third of students were able to correctly differentiate the function using *both* the chain and product rules, while another third correctly employed the product rule, but not the chain rule. The final third of students did not employ either rule of differentiation correctly.

Student difficulties with physics concepts

- *Multiplicity, microstates vs. macrostates confusion*

We have observed and recorded specific student difficulties with concepts related to the statistical interpretation of entropy, including the concepts of statistical uncertainty, multiplicity, and the distinction between a system's microstates and macrostates. Students often enter our statistical physics course with little or no understanding of the nature of statistical uncertainty, particularly with how this uncertainty changes as sample size increases. The fact that this uncertainty decreases with increasing N is a central concept necessary for the complete development of the statistical interpretation of entropy, and explains why the macroscopic world displays so much regularity and predictability. Additionally, we have evidence that students often confuse and/or conflate the two concepts of macrostate and microstate. In questions where students are asked to somehow make a distinction between the two, many fail to see that macrostates are invariably degenerate, that is, there are many microstates associated with a single macrostate. Most textbooks deal with these concepts in a perfunctory manner, with the assumption that such statistics concepts would have already been developed in a prerequisite mathematics course.

- *State functions, reversible vs. irreversible processes*

Several aspects of our work speak to this concept. A great deal of work has been done with student understanding of entropy, including the extent to which students recognize that entropy is a state function when analyzing thermodynamic processes. Students often fail to apply the state function property of entropy, even after instruction. (See discussion of entropy results above.)

In an interview involving free expansion of a gas, several students expressed puzzlement at how the First Law of Thermodynamics relates to irreversible processes. This is an instance of difficulties with appropriate invocation of *state function*. Although the students reasoned that no work was done by the expanding gas, they were confused when they attempted to calculate the work as the integral of PdV, arriving at a nonzero answer. (Students were not given a P–V diagram for this process.)

Other issues with the irreversible free expansion were elucidated by the interviews. Interview subjects were asked several questions about the process, ranging from whether any of their answers would change if the gas were not insulated, to whether the rate of the expansion would play any role in their choice of answer. Responses indicated confusion with the process itself, sometimes even with additional specific information about the initial and final states provided.

We also have some results, from student comparisons of work based on P-V diagrams and integrals on graphs, that students can invoke the state function property to compare quantities, correctly (internal energy change) or incorrectly (work), but that they seem to lack an appreciation of the mathematical property of *function* that complements the physics concept of state function.

- *Material properties*

  See discussion of partial derivatives above
- *Entropy, temperature; the Second Law*

  Mentioned in previous bullets.
- *Adiabatic and isothermal processes*

  Results on student understanding of entropy speak to any anticipated confusion between adiabatic and isothermal processes, possibly due to a functional confusion between heat and temperature. (See discussion of entropy results above.) Very few students assumed that no heat was transferred during an isothermal process, and that an adiabatic process did not result in a temperature change. Students seemed most comfortable with isothermal processes on questions, and almost as comfortable with adiabatic processes, although several students had difficulties with using statistical reasoning to think about the entropy change of the surroundings during an adiabatic expansion.
- *Maxwell relations, properties and meaning*

  See discussion of partial derivatives above
- *Density of States: definitions, interpretation, applications*

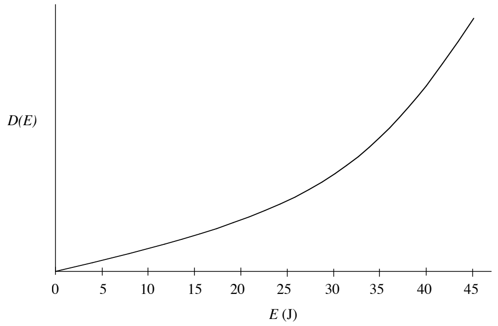
  Data gathered over several semesters of *Statistical Mechanics* reveal that students display multiple difficulties in interpreting the density of states function. This function described the number of microstates available, per unit energy, to a system when it is in a particular energy macrostate. Importantly, this function is meant to be integrated, as it is applicable when the number of microstates is so vast that the multiplicity of the system can be regarded as a continuous function of energy (see figure below). Upon integration, the function yields the *multiplicity* of the given macrostate. Inverting this logic provides an expression for the density of states, $D(E)$, as the derivative with respect to energy of the system multiplicity, ω :

$$D(E) = d\omega /dE.$$

Many students fail to understand the integral nature of this relationship, often simply associating the multiplicity of the system with the value of $D(E)$ evaluated at the system energy E, or by multiplying $D(E)$ by E, or some other combination of $D(E)$ and E.

In Spring 2006 and 2007, we asked our density of states pretest with a slight revision: rather than call the function by its name, we simply described it as the derivative of multiplicity with respect to energy. Interestingly, performance was much higher on this task with this slight change, suggesting to us that if we could motivate this definition of the density of states, a large portion of the student difficulties with the concept might be addressed.

The *density of states function*, *D(E)*, is a function that quantifies the number of ways, for a given unit energy, that individual constituents of a given macroscopic system can be arranged to attain a certain equilibrium system energy state. Presented below is a graph of *D(E)* versus energy *E* for a particular system, where *D(E)* is a known function. When the system is in thermal equilibrium, the mean energy of the system can be measured to be a certain value *E*, with measurements fluctuating about this value by as much as δE.



$$\omega = \int_{E-\delta E}^{E+\delta E} D(E')dE'$$

A graph of the density of states for a certain system, and the relationship between the density of states and multiplicity.

Based on these results we developed and revised two versions of a tutorial titled ***Multiplicity and the Density of States***. One version was deemed too long and rather complicated, while the shorter version was further revised and implemented in a pilot-test of the curriculum in early Spring 2008. (The longer version is currently being edited into several separate tutorials intended to be a sequence of tutorials on this topic, possibly replacing several classes of lecture. The short version of the tutorial is provided at the end of this document.) The implementation was videotaped for analysis. Field notes and observations determined several sticking points for students, which are currently being edited. Once students overcame these points, however, the tutorial appeared to run quite smoothly. We will be receiving student post-test data soon from a mid-term examination and homework assignments, and anticipate analyzing the effectiveness of this tutorial.

- *Quantum gases (e.g., density of BEC)*

On a written question, several students indicate a belief that the density of a BEC is greater than that of the liquid form of the element in question, due to the "closeness" and "inactivity" of the atoms.

Differences in student understanding of thermodynamic concepts across disciplines

As mentioned in *Activities,* we have been able to ask identical written questions in physics, chemistry, and chemical engineering courses in which thermodynamics is taught. We have asked questions dealing with entropy, partial derivatives, and integrals and state functions. While a detailed analysis is ongoing, one preliminary result is that many of the mathematical difficulties seen in physics courses are amplified in chemistry. PI Thompson attended the *19th Biennial Conference on Chemical Education* (Purdue University, August 2006) to present some of these findings and to discuss them with researchers in chemical education, and was subsequently invited to give a seminar in Chemical Education at Purdue in November 2006 on the findings.

Results from the entropy work reveal distinct patterns of specific reasoning in different courses. Some populations tend toward more exclusively statistical explanations, which leads to incorrect responses on some aspects of the questions asked; other groups favor thermodynamic explanations, the success of which also are task-dependent. Students able to fluently use both types of reasoning – and recognize when one is favorable – are more successful on the comprehensive task we asked. The highest overall performance in this vein was by the students in the *Physical Thermodynamics* course and the physics graduate students who were given these questions as part of the comprehensive exam in August 2006.

Supplemental documents for *Project Findings*

- Entropy diagnostic questions (two versions)
- Tutorial on *Entropy changes in ideal gas processes*
- Post-test entropy tutorial question ('the throttling process')
- Tutorial on *Partial derivatives and material properties*
- Calculus diagnostic quiz
- Tutorial on *Multiplicity and the density of states*
- Instructor's guide for tutorial on *Multiplicity and the density of states*
- Pretest on probability and uncertainty

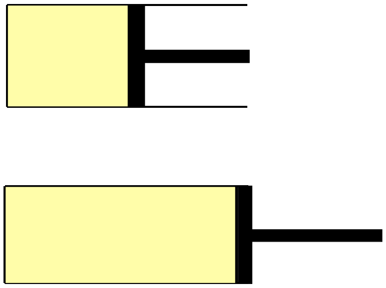
Pretest Version
Administered in *Physical Thermodynamics, Thermal Physics, Chemical Engineering, and Physical Chemistry* samples

1. Consider the two processes described below.

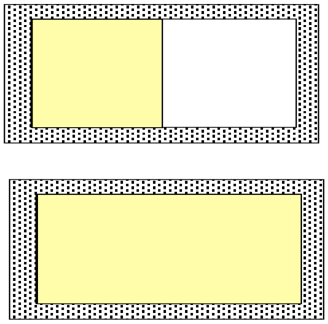
   Process #1: Five moles of an ideal gas are initially confined in a one-liter cylinder with a movable piston, at a temperature of 300 K. Slowly the gas expands against the movable piston, while the cylinder is in contact with a thermal reservoir at 300 K. The temperature of the gas remains constant at 300 K while the volume increases to two liters.

   Process #2: A thin plastic sheet divides an insulated two-liter container in half. Five moles of the same ideal gas are confined to one half of the container, at a temperature of 300 K. The other half of the container is a vacuum. The plastic divider is suddenly removed and the gas expands to fill the container. Because it is a free expansion of an ideal gas (no work is done on or by the gas), the final temperature of the gas is *also* 300 K.

#1: *Isothermal Expansion*



#2: *Free Expansion into a Vacuum*



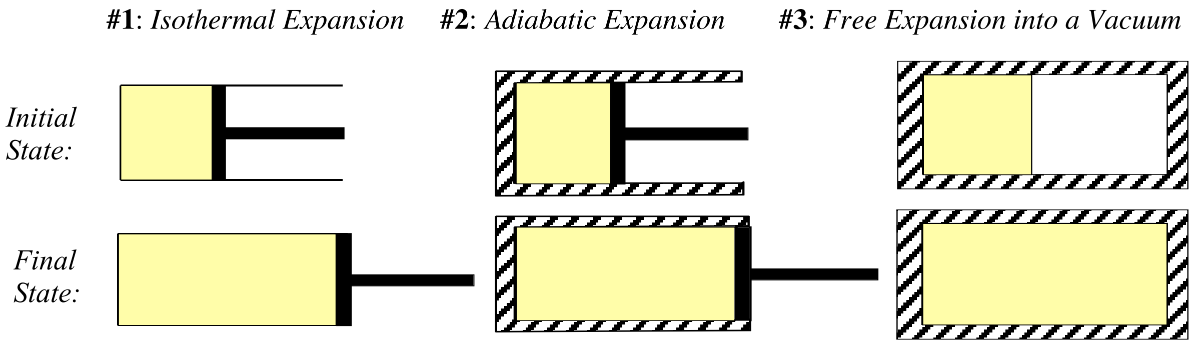
a) Are $\Delta S_{\text{isothermal}}$ and ΔS_{free}, the change in entropy of the **gas** for each process, *positive, negative,* or *zero*? Please explain your reasoning.

b) Is $\Delta S_{\text{isothermal}}$ *greater than*, *less than*, or *equal to* ΔS_{free}? Please explain.

c) Are $\Delta S_{\text{surr-iso}}$ and $\Delta S_{\text{surr-free}}$, the change in entropy of the **surroundings** for each process, *positive, negative,* or *zero*? Please explain.

Post-test Version
Administered in *Physical Thermodynamics (2004 only)* and *Thermal Physics* samples

1. A system consisting of one mole of a monatomic *ideal gas* goes through three different processes as shown below. The initial volume (V_o), pressure (P_o), and temperature (T_o) are the same for each process. Also note that the final volume (V_f) is the same for each process.



For each of the specific quantities listed below,

i. specify whether the quantity is *positive, negative,* or *zero* <u>for *each* of the three processes 1, 2 and 3</u>, and *explain* how you know.

ii. *rank* the values of that specific quantity for each process from greatest to least, keeping in mind that positive values are greater than zero, negative values are less than zero, and a larger negative value is less than a smaller negative value.

a) $\boldsymbol{\Delta U}$, the change in internal energy.

b) $\boldsymbol{W}$, the work done *by* the system.

c) $\boldsymbol{Q}$, the heat transferred *to* the system.

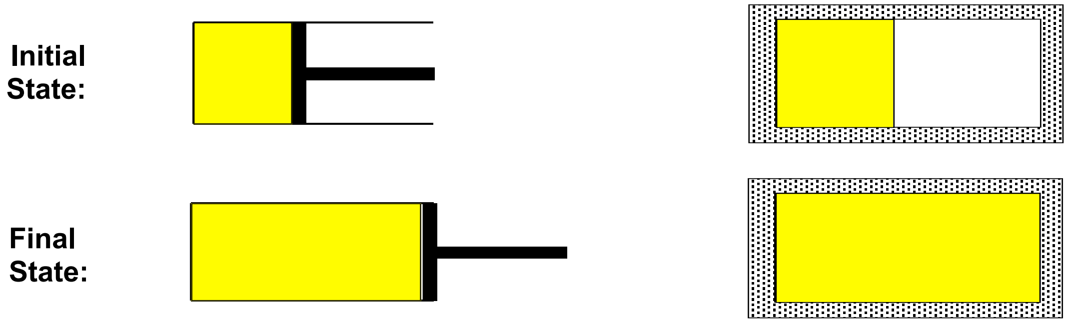
d) $\boldsymbol{\Delta S_{sys}}$, the change in entropy of the **system**

e) $\boldsymbol{\Delta S_{surr}}$, the change in entropy of the **surroundings**

A system consisting of one mole of a monatomic *ideal gas* goes through two different processes as shown below. The initial values of volume (V_i), pressure (P_i), and temperature (T_i) are the same for each process. Also note that the final volume (V_f) is the same for each process.

Process #1 occurs very slowly so that it is always at the same temperature as the surroundings, and the pressure applied to the piston varies. Note that the piston for Process #1 slides without friction. *(Process #1 is reversible.)*

In Process #2, the system is thermally insulated from its surroundings. The gas is initially trapped in one half of the container by a thin partition; the other half of the container contains vacuum. The partition is removed, and the gas quickly fills the rest of the volume.


#1: *Reversible Isothermal Expansion*

#2: *Free Expansion into a Vacuum*

I. The isothermal expansion

A. Consider Process #1: Explain the meaning of "isothermal."

B. During process #1, state whether the following quantities *increase*, *decrease*, or *remain the same*:

   a. temperature

   b. volume

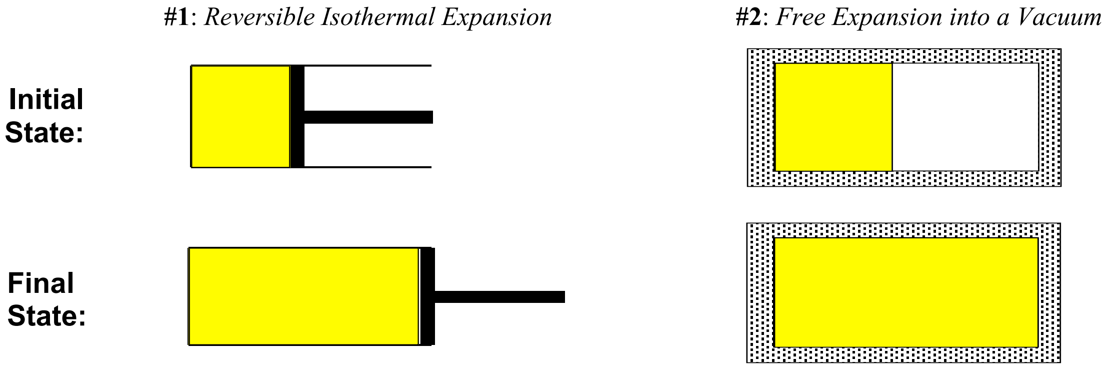
   c. pressure

C. For an ideal gas, internal energy is directly dependent on temperature by the equation $U = \frac{3}{2}nRT$. Does the internal energy of the system in Process #1 (the system consists of the gas only) *increase*, *decrease*, or *remain the same*? Explain.

D. In Process #1, the gas molecules exert a force on the piston by colliding with it while the piston is moving. Does this mean work done by the system on the surroundings is *positive*, *negative*, or *zero*?

E. According to the first law of thermodynamics, is the heat transfer to the system from the surroundings in Process #1 *positive*, *negative*, or *zero*? Explain.

Check that you and your group members have the same answers and consistent explanations for the questions above. If not, reconcile your responses.



II. The free expansion

A. Consider Process #2: According to the information, the system in Process #2 is thermally insulated. Explain what “thermally insulated” means.

B. In Process #2, is the heat transfer to the system from the surroundings *positive*, *negative*, or *zero*?

C. In Process #2, the gas is expanding but there is no (moving) piston for the molecules to collide against . Is the work done by the system on the surroundings *positive*, *negative*, or *zero*? Explain.

D. According to the first law of thermodynamics, does the internal energy of the system in Process #2 *increase*, *decrease*, or *remain the same*? Explain.

E. During this process, state whether the following quantities *increase*, *decrease*, or *remain the same*:

   a. temperature

   b. volume

   c. pressure

III. Comparing the two processes

A. Is the final volume of the system in Process #2 *greater than*, *less than*, or *equal to* the final volume of the system in Process #1? Answer the same question for the initial volumes. *HINT: Check the information at the top of page 1.*

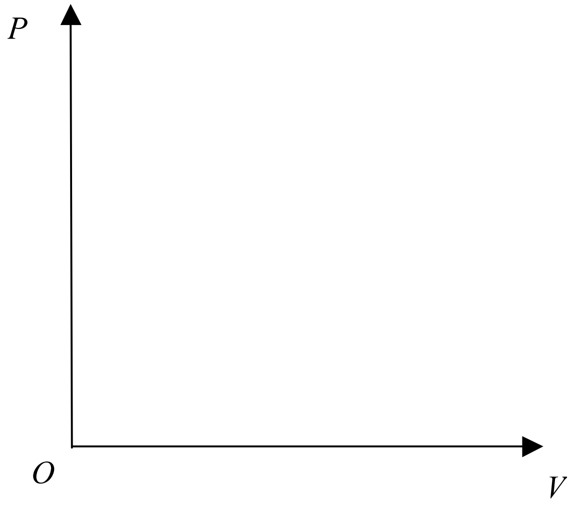
B. Is the final temperature of the system in Process #2 *greater than*, *less than* or *equal to* the final temperature of the system in Process #1? Explain.

C. Is the final pressure of the system in Process #2 *greater than*, *less than* or *equal to* the final pressure of the system in Process #1? Explain.

Check that you and your group members have the same answers and consistent explanations for the questions above. If not, reconcile the responses.

D. Draw points to represent the initial and final states of the two processes on the same P-V diagram; label each state 1_i, 1_f, 2_i, and 2_f, respectively. (e.g. 1_i is the initial state of Process #1, etc.)

Note: Check that the final volumes of both processes are the same.



Is your diagram consistent with your answer to Questions A, B, and C on the previous page?

E. Which process has the greater magnitude of heat transfer to the system? If the two are equal, indicate with an "=" symbol.

IV. Two methods for determining the change in entropy

The change in the entropy of a system that begins in initial state *i* and ends in final state *f* can be expressed as $\Delta S = \int_i^f \frac{đQ_{reversible}}{T}$. Here, $đQ_{reversible}$ represents a small amount of heat transfer to the system during a ***reversible*** process from *i* to *f*; the *T* in this equation represents the temperature of the system during the process.

A. Does the entropy of the system *increase*, *decrease*, or *remain the same* for Process #1?

B. Does the entropy of the system *increase*, *decrease*, or *remain the same* for Process #2?

C. Rank the change in entropy of the system for Process #1 and Process #2. If the two are equal, indicate with an "=" symbol.

Are your answers to Questions A and B consistent with $\Delta S = \int_i^f \frac{dQ_{reversible}}{T}$? Explain.

The change in any state function X during a process from an initial state to a final state can be expressed in the following form: $\Delta X \equiv X_{(\text{final state})} - X_{(\text{initial state})}$.

D. Using the relationship above, write an expression for the change in entropy during an ideal gas process.

E. Compare the initial states of the two processes (recall the info at the top of page 1), and the final states of the two processes (recall your responses to Questions A, B, and C in Part III).

F. Is the analysis above consistent with your response to Question C? Explain why or why not.

G. Is it possible to write down *meaningful* similar expressions for the work done by the gas, and the heat transfer during the process? If so, write down these expressions. If not, explain why such expressions are not meaningful.

Consider ΔS_2 and ΔS_1, the *changes* in the entropy of the system during Process #2 and Process #1, respectively; $\Delta S \equiv S_{(\text{final state})} - S_{(\text{initial state})}$. Three students are discussing whether ΔS_2 is *greater than*, *equal to*, or *less than* ΔS_1. Read through the discussion and follow the directions below.

> **Student A:** "*I think that the entropy for Process #2 is going to stay the same. The system is thermally insulated so if there is no heat transfer to the system from the surroundings there is no change in the entropy of the system because* $\Delta S = \int_i^f \frac{đQ_{reversible}}{T}$."
>
> **Student B:** "*That makes sense from that ΔS equation we were given, but can we even use that equation if this is not a reversible process? Entropy is like pressure and volume – it depends on the state of the system. I mean, Process #2 has the exact same final pressure, volume, and temperature as Process #1, so I think that the entropy in Process #2 will increase by the same amount that entropy in Process #1 increases.*"
>
> **Student C:** "*Couldn't we just push the gas back to its original state in Process #2? Wouldn't that make it reversible?*

H. Re-read each student's statement and comment on the parts with which you agree, and among your group identify any statements that you believe are incorrect. Explain your reasoning.

V. Calculating entropy changes for irreversible processes

Student *B* provides a useful insight into comparing entropy changes between reversible and irreversible processes. However, Student *B* also points out that the ΔS equation provided cannot be used to calculate irreversible processes. Extend Student *B*'s insight into a method for calculating entropy changes for ***irreversible*** processes.

Discuss your reasoning and that of your group with the recitation instructor before continuing.

Tutorial Homework

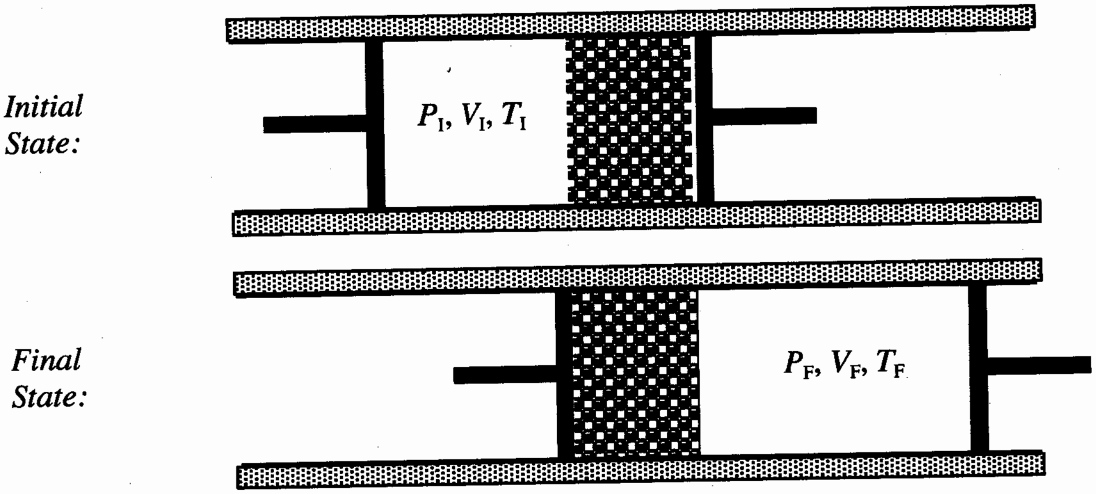
1. Determine two alternate processes or process combinations by which one can explicitly calculate the change in entropy during the free expansion labeled Process 2.

2. Suppose the final volume of the gas in Process 2 is twice the initial volume, i.e. $V_f = 2V_i$. Assuming that the ideal gas is monatomic, show that all three paths (the isothermal expansion, and the two processes or process combinations that you chose) have the same change in entropy.

3. A 2-mole sample of a *diatomic* ideal gas is in an initial state with a pressure of 25 atm and a volume of 2 liters. The gas undergoes an irreversible process, ending in a final state with a pressure of 30 atm and a final volume of 4 liters. Calculate ΔS for this process. *Explain your method and show your work.*

   $(R = 0.08206 \dfrac{liter \cdot atm}{mol \cdot K})$

3. An insulated system consisting of two kilomoles of a diatomic ideal gas undergoes a throttling process by being forced through a porous plug, shown below. The ratio of the initial pressure to the final pressure is 3 atm to 1 atm, and the initial temperature of the gas is 25° C.



The determination of the value of the Joule–Thomson coefficient, $\mu = \left(\frac{\partial T}{\partial P}\right)_H$, was the experimental outcome of the Joule–Thomson experiment utilizing such a throttling process as described above.

a) Is a throttling process *reversible* or *irreversible*? Explain.

b) Does the enthalpy of the gas *increase*, *decrease*, or *remain the same* during the throttling process? Briefly explain your response.

c) Determine the final temperature T_F of the gas.

d) Draw (to scale) the initial and final states of the throttling process on a *P-V* diagram.

e) Determine the entropy change of the gas during the throttling process. Explain your method and result.

Previously, we learned how one can form a *total differential* of a thermodynamic variable known as a *state function*. For instance, a general state function R of two variables, i.e. $R(B, C)$, has a total differential of the form

$$dR = XdB + YdC. \quad (1)$$

Review: Interpret the above equation to determine expressions for X and Y in terms of the variables R, B, and C. Give a physical interpretation for these expressions (explain in words the process that these mathematical expressions describe.)

In this tutorial, we will be studying certain variables that belong to the total differential of the state function of *volume*.

I. Total differential of volume

A. The Ideal Gas equation of state relates the three variables P, V, and T in a closed system, i.e. no change in n. How many variables can you *simultaneously* set to arbitrary values? Please explain.

A variable that you can set to an arbitrary value is called an *independent variable*.

How many variables are there whose value *depends* on the values of the independent variables? Does it matter which, if any, variable is chosen to depend on the values of the other variables? Explain.

A variable that depends on the value of the independent variables is a *dependent variable*.

B. In an experiment, suppose you are measuring how the volume of a fixed amount of ideal gas changes when you change the pressure of the system at constant temperature. Which of the variables are *independent*, and which are *dependent*? Briefly explain.

Let's choose V to be our dependent variable for now (there are often good physical/experimental reasons for this choice). Fill in the following blanks, then explain the expression:

$$V = V(\_\_,\_\_) \tag{2}$$

Now form the total differential of volume. Remember, n is fixed.

What do the coefficients tell you? Express the meaning of the coefficients in sentences.

C. You have previously studied the *isothermal compressibility* of a substance, referred to by the symbol κ. κ is explicitly defined as:

$$\kappa \equiv -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T . \tag{3}$$

Additionally the *thermal expansivity* of a substance, β, is defined as:

$$\beta \equiv \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P . \tag{4}$$

Why is there a negative sign in the expression for κ, but not in the expression for β?

Rewrite your expression for the total differential of volume (as in I, B), but this time use κ and β.

II. Derivatives of material properties

Consider the following question:

$$\text{“Show that in general } \left(\frac{\partial \beta}{\partial P}\right)_T + \left(\frac{\partial \kappa}{\partial T}\right)_P = 0.\text{”} \qquad (5)$$

A. Before working through any of the steps, several students begin by discussing a possible solution to the problem.

Student 1: “The two derivatives are both equal to zero, so they have to add to zero. In the second term, you’re taking the derivative with respect to T*, but* T *has already been held constant in the first derivative in the definition of isothermal compressibility. So you’re taking the derivative of a constant, which is zero. It just follows from the definition – ‘isothermal’ compressibility.”*

Student 2: “I see, and it’s the same for the expansivity too, you’re differentiating β *with respect to* P *after you’ve already held* P *constant to get it in the first place.”*

Do you agree or disagree with these students’ reasoning? Elaborate.

B. *Working individually,* perform the necessary differentiation to determine the expressions for each partial derivative in equation (5).

Discuss your expressions with your group. Make sure everyone is in agreement on the correct form of the expressions. Make sure you have included both the *product rule* and the *chain rule* in your differentiation.

Do not proceed any further until you have checked your work with an instructor.

C. Once you’re satisfied with the differentiation, write out all the terms in equation (5) here:

Now compare notes with the students.

Student 1: *"So I guess it's a little more complicated than I said originally. One of the terms of the two derivatives contain only first partial derivatives and are equal and opposite, so when you add them together you get zero. The other terms contain second partial derivatives of volume with respect to both P and T, and* ***they*** *are both zero for the reasons I mentioned earlier."*

Student 2: *"But they look so similar, one just has a negative sign in front of it and the order of differentiation is different. Could they be equal and opposite too, like the first terms? Then they wouldn't have to equal zero, but the whole expression still adds to zero."*

Student 3: *"I don't know. I liked the idea that the original two derivatives were each equal to zero, but now we've seen that at least the first terms are not equal to zero, and the second terms may not be zero either. So what's up?"*

Comment on the reasoning provided by each student. With which student(s), if any, do you agree?

At this point, we may need to appeal to a higher mathematical authority to clear things up. (Not for long though: you'll be able to prove the following theorem in your homework assignment for next class period.) Consider the following theorem, attributed to the 17th-century mathematician Alexis Clairaut:

> *For a function with continuous and defined second partial derivatives,*
> *the* ***mixed*** *second partials of the function are equal.*

D. Does this theorem clear up the issues the students are having? With the aid of this theorem, present the final solution to the question asked in (5) above.

E. Do you think all the students would be satisfied with the solution now? Are *you* satisfied with the solution now? Explain why or why not.

Please stop at this point. We will resume with part III in the next class session.

Tutorial Homework Problem

(*to be brought to the next class period for the conclusion of the tutorial)*

Proof of Clairaut's Theorem.

Using the mathematical definition of a derivative provided below, show that the second mixed partials of a state function are equal.

$$f'(x) = \frac{df}{dx} \equiv \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

III. Graphical interpretation of mixed second partials

In this section we will explore what it means for a function to have ***nonzero*** *and* ***equal*** mixed second partials by reasoning about the situation graphically.

Ask your instructor for a graphical depiction of the *P-V-T* surface of an ideal gas (the instructor may also have a 3-D model of the same surface at the front of the room). You should refer to these surfaces in completing this section of the tutorial.

A. With two different colors of ink (or pencil), draw and identify the following features on the surface at point *a*. For each expression, explain in words what these features represent graphically.

i. $\left(\frac{\partial V}{\partial P}\right)_T$ ii. $\left(\frac{\partial V}{\partial T}\right)_P$

Before you check this on the graph, do you expect the value of either of these two derivatives to change for different values of *pressure*, or not? Explain.

Before you check this on the graph, do you expect the value of either of these two derivatives to change for different values of *temperature*, or not? Explain.

B. Identify on the *P-V-T* diagram the same two derivatives given in part A, only now at points *b* and *c* instead of at *a*.

Do each of these two *derivatives* change as you move along the variable with respect to which they are differentiated? If so, how?

Do each of these two *derivatives* change as you move along the variable that is held constant during differentiation? If so, how?

C. Obtain a graph of the projection of the ideal gas *P*-*V*-*T* surface onto the *V*-*T* plane from your instructor. Identify $\left(\frac{\partial V}{\partial T}\right)_P$ at temperature T_2 for the three different values of pressure depicted.

Does $\left(\frac{\partial V}{\partial T}\right)_P$ at temperature T_2 *increase, decrease,* or *remain the same* as you go from lower to higher gas *pressures*? Explain what this means physically. Does it make sense to you?

Is this consistent with your responses in part B of this section?

D. Obtain another projection graph from your instructor, this one the projection of the *P*-*V*-*T* surface onto the *V*-*P* plane. Identify $\left(\frac{\partial V}{\partial P}\right)_T$ at pressure P_2 for the three different values of temperature depicted.

Does $\left(\frac{\partial V}{\partial P}\right)_T$ at pressure P_2 *increase, decrease,* or *remain the same* as you go from lower to higher *temperatures*? Explain what this means physically. Does it make sense to you?

Is this consistent with your responses in part B of this section?

E. Compare how, if at all, the two derivatives in parts C and D change (i.e., compare the *signs* of the changes).

Can you say anything about the *magnitude* of the change at this point?

F. Provide a graphical interpretation of a mixed second partial derivative. (Hint: include the concept of *slope* in your interpretation.) Be sure to include an explanation as to why mixed second partials are in general *not* equal to zero.

Explain what Clairaut's theorem says about both the *sign* and the *magnitude* of the changes of the derivatives in C and D, using your graphical interpretation.

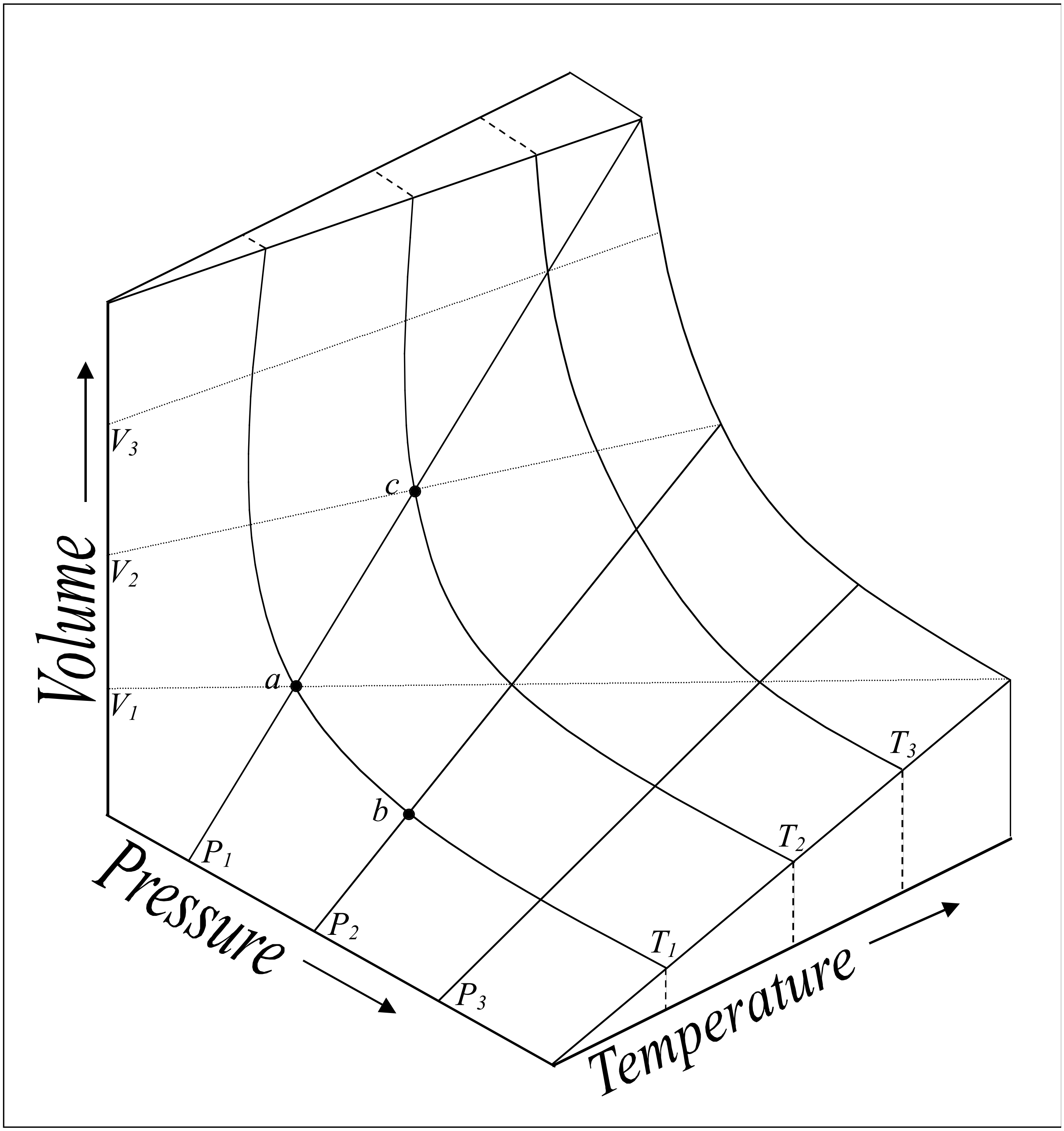


Figure 1. P-V-T surface for an ideal gas with fixed n. Surface obeys equation $PV=nRT$.

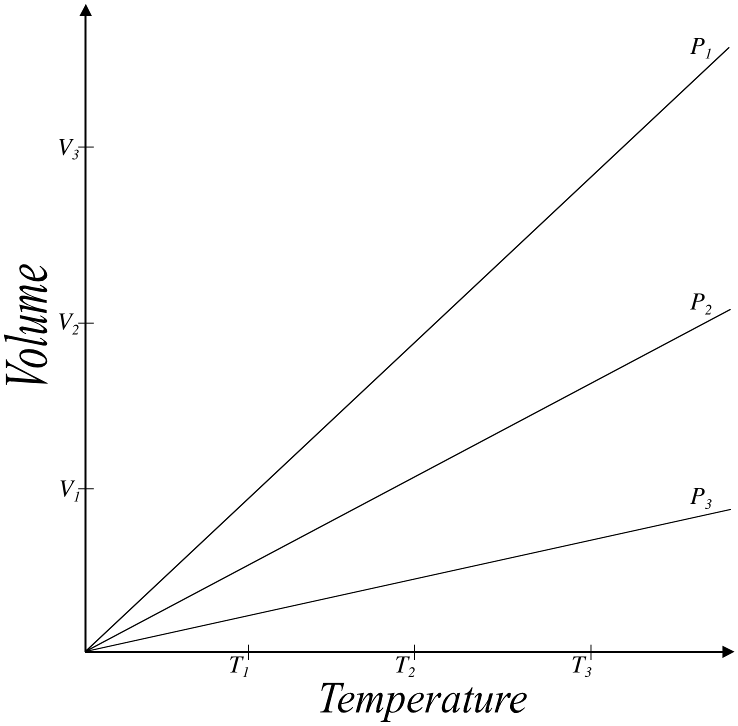


Figure 2. *V-T* projection of an ideal gas *P-V-T* surface with fixed *n*.

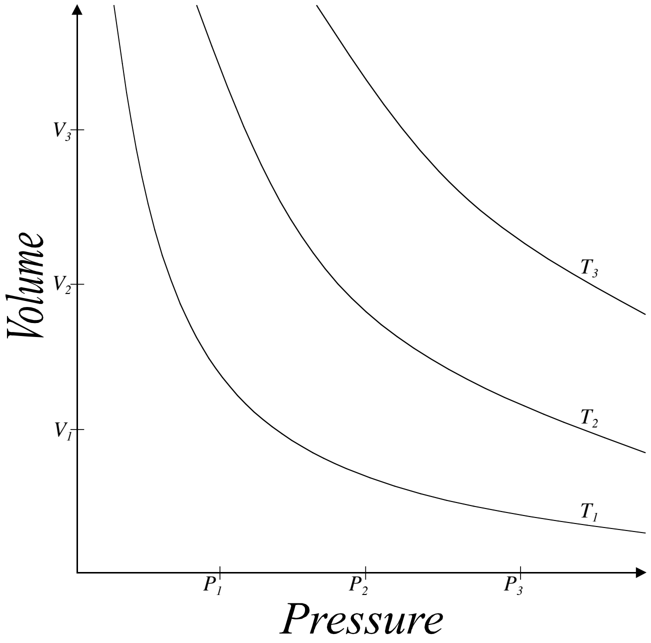


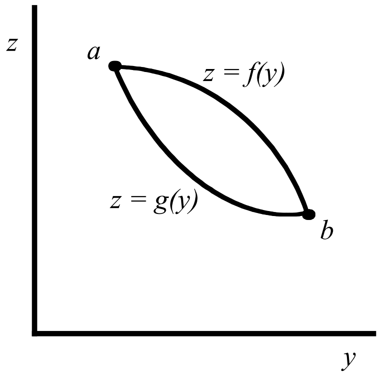
Figure 3. *V-P* projection of an ideal gas *P-V-T* surface with fixed *n*.

MAT 228 Name:______________________

Fall 2007 *Sec 001*

1. Two functions have been graphed on the *y*-*z* graph shown at right, and are labeled *f(y)* and *g(y)*. Both functions start at point *a* and end at point *b*.

   Consider the integrals $I_1 \equiv \int_a^b f(y)dy$ and $I_2 \equiv \int_a^b g(y)dy$.

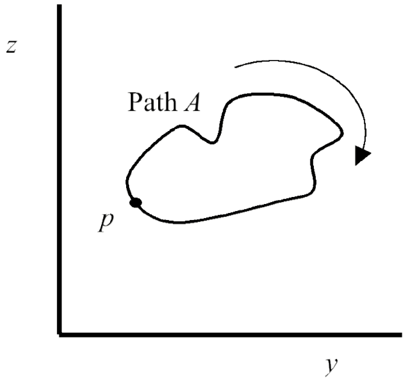


   a) Is the integral I_1 *positive*, *negative*, *zero*, or is there *not enough information to decide*? Please explain your reasoning.

   b) Is the integral I_2 *positive*, *negative*, *zero*, or is there *not enough information to decide*? Please explain.

   c) Is the absolute value of the integral I_1 *greater than, less than, or equal to* the absolute value of the integral I_2, or is there *not enough information to decide*? Please explain.

2. H is a function of the independent variables z and y; i.e., $H = H(z, y)$. A path has been traced out on the y-z graph at the right, and has been labeled Path A.



Consider the closed path integral

$$I_1 \equiv \oint_{A,clockwise} z\,dy\,,$$

where the path starts at point p and proceeds <u>clockwise</u> about Path A until reaching point p again.

a) Is the integral I_1 *positive*, *negative*, *zero*, or is there *not enough information to decide*? Please explain your reasoning.

Refer again to the graph in part (a). Consider the closed path integral

$$I_2 \equiv \oint_{A,clockwise} dH\,,$$

where the path starts at point p and proceeds <u>clockwise</u> around Path A.

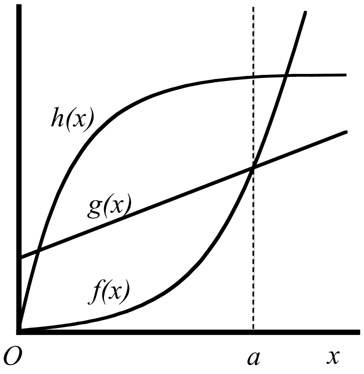
b) Is the integral I_2 *positive*, *negative*, *zero*, or is there *not enough information to decide*? Explain.

3. Z is a function of the two variables x and y, i.e. $Z = Z(x,y)$. Consider the following two expressions:

$$\alpha = -\frac{1}{Z}\frac{\partial Z}{\partial x} \quad \text{and} \quad \beta = \frac{1}{Z}\frac{\partial Z}{\partial y} \; .$$

Show that in general $\dfrac{\partial \alpha}{\partial y} + \dfrac{\partial \beta}{\partial x} = 0$. Explain your reasoning.

4. Three functions have been graphed on the graph shown at right, and are labeled $f(x)$, $g(x)$, and $h(x)$.

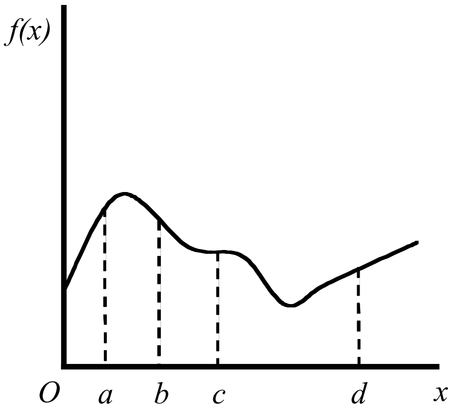


Consider the derivatives $\left.\dfrac{df}{dx}\right|_{x=a}$, $\left.\dfrac{dg}{dx}\right|_{x=a}$, and $\left.\dfrac{dh}{dx}\right|_{x=a}$

a) For each of the derivatives listed above, state whether the derivative is *positive*, *negative*, *zero*, or is there *not enough information to decide*? Please explain your reasoning.

b) *Rank* the absolute values of the three derivatives using the following possible terms: *greater than* or *equal*. If there is *not enough information to decide, please say so explicitly*? Explain your reasoning.

5. *f* is a function if the variable *x*, i.e. $f = f(x)$. Consider the graph of $f(x)$ versus *x* shown on the right.



   Rank the value (not absolute value!) of the *slope* of $f(x)$ at the four points *a, b, c, d* from *greatest* to *least*, keeping in mind that positive values are greater than negative values, and that a larger negative value is less than a smaller negative value. If two slopes are equal, state this explicitly. If there is *not enough information to decide*, state so explicitly. Explain your reasoning.

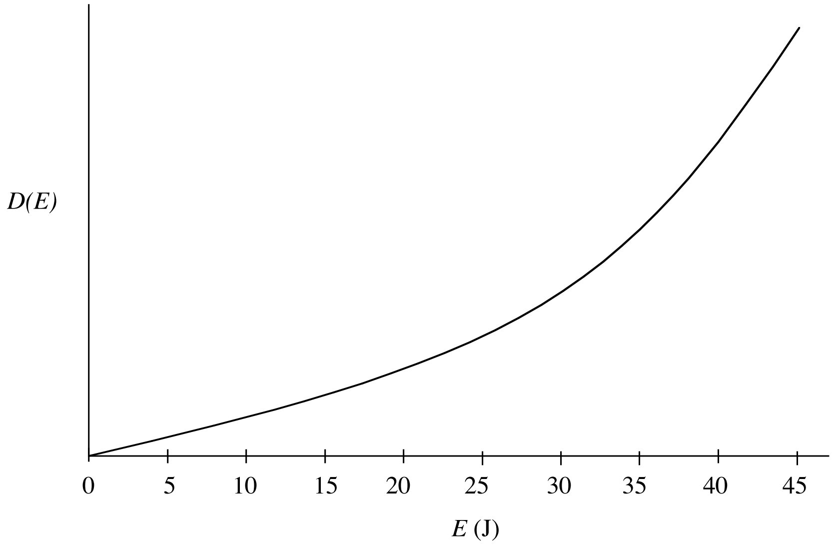
6. The functions $R(x)$, $A(x)$ and $B(x)$ are all functions of the variable *x*. Find the derivative of *R* with respect to *x* where $R(x) = A(x) \bullet (B(x))^2$.

Multiplicity and the Density of States

I. The density of states: an introduction

(from Baierlein, p. 75) When a physical system has reached thermal equilibrium, its macroscopic properties do not change over time (apart from minor fluctuations). Quantum mechanics tells us that *energy* states of an isolated system provide predictions and estimates that are constant in time; therefore, such states are appropriate for a microscopic description of thermal equilibrium. (Of course, the fact that internal energy is a *state function* also tells us this.)

The *density of states function*, *D(E)*, is a function that quantifies the number of ways, for a given unit energy, that individual constituents of a given macroscopic system can be arranged to attain a certain equilibrium system energy state. Presented below is a graph of *D(E)* versus energy *E* for a particular system, where *D(E)* is a known function. When the system is in thermal equilibrium, the mean energy of the system can be measured to be a certain value *E*, with measurements fluctuating about this value by as much as δE.



A. What are the units of *D(E)?*

B. Describe the behavior of *D(E)* as observed in the graph. *Conceptually*, what does this behavior tell you about the system as its energy increases? Be sure to include the concept of “microstate” in your description.

C. Without knowing the value of E, is it possible to determine the equilibrium state energy of the system from this graph? If so, explain why and provide the equilibrium state energy. If not, explain why not.

II. Connecting the density of states with multiplicity

Suppose that for our particular system, which is in thermal equilibrium, the mean energy of the system is measured to be 25 J, with measurements fluctuating about this value by as much as 2.5 J.

A. Given the information above, what does it mean for the system to be in this particular macrostate (the "$E = 25$ J macrostate")?

B. Based on your above response, provide a description of the microstates that constitute the "$E = 25$ J macrostate". Can you think of a way to count all of these microstates? What would this procedure tell you?

C. Working alone*, determine* a mathematical expression for the multiplicity, ω, of the system in this equilibrium state based on the description of *D(E)* on the previous page. Be sure to explain your expression in words as well as symbols. Once you have determined your individual expression, compare it with those of your group members. Discuss any discrepancies.

D. Consider the following student discussion:

Student 1: “We’re looking for the multiplicity of the system when it has an energy of 25 Joules. I think we should integrate the density of states function $D(E)$ with respect to dE from 0 to 25 Joules. That should give us the multiplicity of the equilibrium state.”

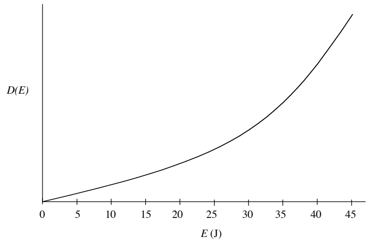
Student 2: “You’re thinking about this way too hard. We *already* know the number of microstates as a function of energy, it’s just $D(E)$. So the value of $D(E)$ at $E = 25$ Joules *has* to be the multiplicity of the equilibrium state. There’s your answer: $\omega = D(E{=}25\text{ J})$.”

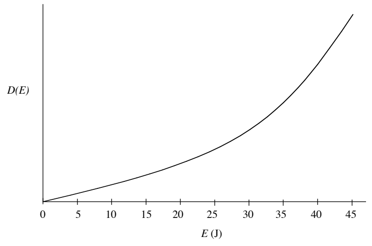
Student 3: “But that doesn’t work dimensionally. Multiplicity can’t have dimensions; it’s just a number. To get rid of the J^{-1}, we need to multiply $D(E{=}25\text{ J})$ by the energy E, which is also 25 J. So I think $\omega = D(E{=}25\text{ J}) \times 25\text{ J}$.”

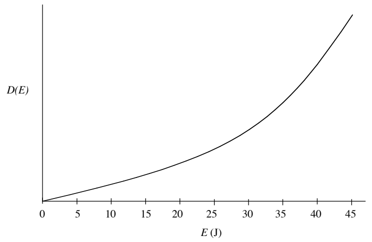
Student 4: “But what about the fluctuations around the equilibrium energy? Maybe we should multiply $D(E{=}25\text{ J})$ by 2.5 J, or even by 5 J to take care of the whole range.”

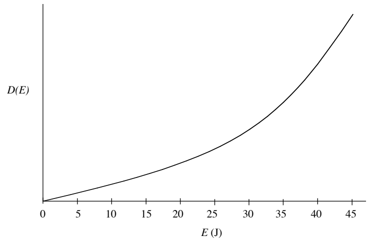
Each of these students has incorrect reasoning, although some have more than others. Explain why each is incorrect and point out the particular bit of reasoning left out by *each* student.

The graph on page 1 has been reproduced four times, shown below. On a separate graph for each student, provide a graphical interpretation of each of the above students’ expressions.



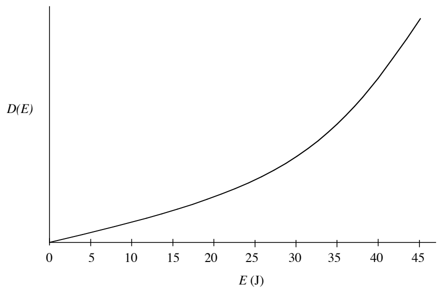






E. Once you and your group members have come to a consensus on an expression for the multiplicity of the system in an equilibrium state, write it down below in its most general form. Make sure you can point out where each of the following features appears in your expression:
   - i) *D(E),*
   - ii) *E,*
   - iii) δE, and
   - iv) The 'units' of multiplicity.

On the graph below, provide a graphical interpretation of your above expression for the "*E* = 25 J macrostate".



F. Based on your expression, what variable(s) is(are) ω a function of? Explain.

G. If you knew ω in its complete functional form of the above variables, how then could you find *D(E)?* In other words, write an expression for *D(E)* in terms of ω.

STOP! Do not proceed past this point until checking your expression/reasoning with an instructor.

III. An expression for the density of states of an ideal gas

Now that we have explored the concept of density of states in general, it's time to find this function for a real (or at least less contrived) example: an ideal gas.

A. Besides energy, what other variables might *D(E)* depend on for an ideal gas? Explain.

B. Based on what you already know, write an expression for the multiplicity of an ideal gas of *N* particles. (It's okay to have a general constant of proportionality in your statement.)

Working alone, use your above expression for ω to determine *D(E)* for this ideal gas. Again, it's okay if you have some undetermined constant; we really just want to explore the energy dependence of the density of states.

Compare your answer to those of your group members. Explain any discrepancies.

C. Based on your previous expression, determine *D(E)* for a single ideal gas particle. Explain qualitatively how the behavior of *D(E)* for this system differs from that of a large sample of ideal gas. Provide a rationale for this difference.

D. Compare the determined *D(E)* for a single ideal gas particle to the density of states function for a single particle derived in Baierlein's text (Equation 4.11, page 78). In particular, explore the nature of your undefined constant. Check your response to part A in this section with this expression.

Instructor's guide for ***Multiplicity and the density of states***

I. Density of states: an introduction

We want students to explore the particular form of *D(E)* provided here. What are its units, what does the graph tell us about number of microstates for a given energy value as energy increases.

I.C. We want students to see it is not possible to determine an equilibrium state from *D(E)*, as it gives the number of microstates as a function of equilibrium energy values.

II. Connecting the density of states with multiplicity

Here we try to motivate a broader description of a macrostate as containing a spread of macrostate energies, rather than a single value. This fluctuation is <u>not</u> the result of measurement error, but is rather an unavoidable feature of any physical system being studied (natural fluctuations, 'noise', etc.). Once this broad macrostate is defined, it is connected to a similarly broadened concept of multiplicity. This prompts an expression for multiplicity in terms of an integral of *D(E)*. A student discussion solidifies the correct expression by showing various incorrect ones. The integral nature of the expression is strengthened by having students construct graphical interpretations of various expressions (area under curve should be activated here!). Finally, students invert their reasoning to determine an expression for *D(E)* in terms of multiplicity, specifically dw/dE.

II.A. "If the system is measured to have an energy anywhere between 22.5 J and 27.5 J, we say it is in the E=25 J macrostate."

II.B. "All microstates that contribute to macroscopic energies between 22.5 J and 27.5 J are microstates of the E=25 J macrostate. The sum of these is the multiplicity of the macrostate."
** A continuous sum => Integral! **

II.E.
** Have students decide which incorrect student has the closest graphical interpretation to the correct one. Use this to scaffold an appropriate approximation for ω using *D(E)* and δE. **

II.G.
** Hint: think antiderivative! **

III. An expression for the density of states of an ideal gas

This section is much like the homework problem (Ch. 4) where they find the $E^{3N/2}$ dependence of the gas, just in tutorial form. We want them to be able to easily construct the density of states from a multiplicity equation (of the form $\omega = C(N)\, V^N\, T^{3N/2}$), and we want them to be able to interpret the different behavior for different *N*'s.

III.C. We think of the large *N* graph behavior as the result of a combinatoric combination of *N* single particle graphs. There are <u>so</u> many ways to get a macroscopic *E* using *N* particles, each with individual microstate spreads of $D(\varepsilon)$.

For both of these questions, estimate *all* of your answers as x = __a__ ± __Δa__ .

That is, give your best numerical *answers* for both (a) ***and*** numerical estimates of the *uncertainties* (the ± Δa) that indicate your confidence level in the precision of your answers (*be realistic*).

1. If you flip one coin n times, estimate the value of and the uncertainty of the number of 'heads' that would occur for:

   a) $n = 4$

   b) $n = 100$

   c) $n = 1000$

   d) $n = N_A = 6.022 \times 10^{23}$

   e) Explain the reasoning for your estimates in (a) – (d) above.

2. Suppose you place 1000 identical coins in a large covered box, shake it vigorously, then place the box on a table and open the top. Estimate the value of and the uncertainty of the number of coins that would be lying 'heads'-side up. Explain your estimate.

3. The groundskeeper at the Penobscot Valley Country Club wants to know the total amount of rain (in kg H_2O) that falls on the golf course during a predicted downpour. Before the storm, four atmospheric science majors report to the golf course with timepieces and rain gauges in hand; Andy brings one rain gauge, Betsy brings four, Charlie brings 40, and Debby brings 400. You may assume all know how to use them.

   a) Which student do you expect will be able to determine a value closest to the actual total amount of rainfall? Please explain your reasoning.

   b) *Rank* the uncertainties (as a percentage of the total amount of rainfall) associated with each student's determined value. If any uncertainties are equal, state that explicitly. Explain.

Experiments and Observations

1. *Design, administration, and analysis of written questions*
   - Pretests
     - Design of over 20 written questions dealing with topics throughout thermodynamics and statistical mechanics
     - Data-driven modification of some of the original 20 or so pretests dealing with as many different topics
     - Development of new pretest dealing with student understanding of *equilibrium state*
     - *Metal in Ocean* pretest (from collaborators Meltzer and Christensen) updated for upper-level and administered
     - Administration of pretests to >120 students at U. Maine as well as 5 other universities
     - Analysis of pretest data (see *Findings*)
   - Post-tests
     - Development of post-tests based on pretest findings; given at UMaine as well as several other universities
     - Some pretest questions asked in Year 3 after instruction in course rather than before instruction
     - Development of questions to assess effectiveness of curricular material implementation (tutorials on *Partial derivatives and material properties* and *Entropy*)
     - Administration: post-tests of 15+ pretest topics administered as 34 exam questions
     - Homework assignments for U. Maine physics courses routinely scanned
     - Analysis of examination and relevant homework questions (see *Findings*)
   - Special question: Administered set of questions about the mathematical concepts used in thermodynamics, in a purely mathematical context, to ~100 students at end of Calculus III course at U. Maine in Fall 2007. (Plan to administer to Spring 2008 class also.)

2. *Interviews:* conducted and analyzed 8 clinical interviews of students to follow-up on pretest topics and responses (videotaped)
   - Entropy and 2nd Law ideas in context of ideal gas processes (Six interviews; Brandon Bucy conducted)
   - State functions and partial differentiation in context of material properties (Two interviews; Brandon Bucy conducted)
   - Mathematical conceptual understanding related to P-V diagrams; subjects were students in *Mathematical Methods in Physics* and *Physical Thermodynamics* courses. (8 interviews; Evan Pollock conducted, with help from John Thompson and Brandon Bucy)
3. *Dissemination:* Administration of assessment instruments (pre- and post-tests) among students in 4 different courses as well as graduate students, involving U. Maine and 8 other universities.
   - Courses investigated
     - pure macroscopic thermodynamics
     - statistical physics

    - thermal physics (macro thermo + stat mech)
    - chemical engineering thermodynamics
    - AP chemistry teacher workshop in central Maine
    - physics graduate students taking the comprehensive exam
- Universities involved, with colleagues listed
    - California St. U. – Fullerton (CSUF) – Michael Loverude
    - Iowa St. U. (ISU) – Warren Christensen (part of original project)
    - Seattle Pacific U. (SPU) – Hunter Close
    - U. New Hampshire (UNH) – Dawn Meredith and Bill Hersman (instructor)
    - U. Washington (UW) – David Meltzer (Collaborating PI on original project)
    - Pacific U. – Stephen Hall
    - Southern Illinois University Edwardsville – Rebecca Lindell
    - Augusta State University (Georgia) – Trinanjan Datta

4. *Instructional materials development:* We have identified at least 20 curriculum targets for development. These materials are written in the style of *Tutorials in Introductory Physics* (McDermott, Shaffer, and the Physics Education Group at the University of Washington) and are small-group, conceptually-oriented, guided-inquiry exercises that students work through in class with instructor facilitation.
    - Materials that have been written, tested and revised
        - ***Partial Derivatives and Material Properties***
            - Main goal is to address student difficulties with recognizing equality of mixed second partial derivatives, especially as pertains to material properties (thermal expansivity, isothermal compressibility) and the Maxwell relations
            - Includes a section guiding students to review the concept of total differential (using volume as the function)
            - Uses a graphical representation (P-V-T surface) to guide students to recognize geometrical interpretation of partial derivatives, and of mixed second-order partial derivatives
        - exact differentials, state functions & integrals
        - ***Multiplicity and the Density of States*** (see #5 below)
        - calculating entropy changes in ideal gas processes (see #5 below)

5. *Instructional materials administration:*

We pilot-tested a set of materials titled ***Partial Derivatives and Material Properties*** in the *Physical Thermodynamics* course in Fall 2006 and Fall 2007.

    - Video data, field notes of groups working through tutorial
    - Made revisions to tutorial based on in-class observations of implementation
    - Administered pre- and post-test questions to assess effectiveness of instruction

We pilot-tested a tutorial titled ***Entropy Changes in Ideal Gas Processes*** in the *Physical Thermodynamics* course in Fall 2007. This tutorial was originally developed by Christensen and

Meltzer at Iowa State for the introductory course. We have modified it to use in upper-level course, and included more about entropy as a state function in the tutorial.

  - Developed post-test question to assess effectiveness of instruction
  - Recorded video data and took field notes of groups working through tutorial
  - Administered pre- and post-test questions to assess effectiveness of instruction

We pilot-tested a set of materials titled ***Multiplicity and the Density of States*** in the *Statistical Physics* course in early 2008.

  - Recorded video data and took field notes of groups working through tutorial
  - Administered pre- and post-test questions to assess effectiveness of instruction

In addition to pilot testing our own tutorials, we site-tested a tutorial developed by colleague Michael Loverude (CSUF) titled ***Counting Microstates*** in the *Statistical Physics* course in early 2008.

  - Took field notes of groups working through tutorial
  - Administered pre- and post-test questions to assess effectiveness of instruction

Presentations

- 14 talks (4 invited) and 14 posters (2 invited) at national conferences on physics, physics education, and physics education research, and chemical education research
- 2 talks and 6 posters at 3 regional meetings of AAPT and APS
- 5 invited seminars and colloquia at universities (U. Maryland, U. Maine, Purdue U., Kansas State U., Rochester Inst. of Technology (after grant expires, but based on grant work)

Invited presentations (9 oral, 2 poster)

- Physics Education Research Seminar, University of Maryland, College Park, MD, February 2006, "Are they constant or are they fixed? Student difficulties with partial derivatives in thermodynamics," J.R. Thompson
- American Physical Society April Meeting 2006 (national), Dallas, TX, "Investigating student understanding in advanced thermal physics courses," J.R. Thompson
- *Integrating Science and Mathematics Education Research into Teaching,* The University of Maine, Orono, ME, June 2006, "Investigations of student understanding of thermal physics in the upper division," J.R. Thompson
- 2006 Summer National Meeting of the American Association of Physics Teachers (AAPT), Syracuse U., Syracuse, NY, July 2006: "Seeing what works: An empirical approach to PER," J.R. Thompson, invited poster for "Physics Education Research from Different Perspectives: Why Bother?"
- 2006 Physics Education Research Conference, Syracuse U., Syracuse, NY, August 2006: "Thermal physics as a context for investigating student use of multivariable calculus." J.R. Thompson, D.B. Mountcastle, B.R. Bucy, invited Targeted Poster for "Physics Education Research Across Disciplinary Boundaries"
- Purdue University Chemical Education Seminar, Purdue University, West Lafayette, IN, November 2006, "Investigations of upper-division student understanding of thermodynamics," J.R. Thompson

- 2007 Winter National Meeting of the AAPT, Seattle, WA, January 2007, "Investigating student connections between mathematics and thermal physics," J.R. Thompson
- University of Maine Physics & Astronomy Colloquium, U. Maine, Orono, ME, April 2007, "Investigating student use of mathematics in thermal physics," J.R. Thompson
- Kansas State University Physics Department Colloquium, Manahattan, KS, April 2007, "Investigating student use of mathematics in thermal physics," J.R. Thompson
- 2008 Winter National Meeting of the AAPT, Baltimore, MD, January 2007, "Research on the learning and teaching of thermal and statistical physics," J.R. Thompson

presentations given after the grant period, but based on work done during the grant duration

- Rochester Institute of Technology Physics Department Colloquium, Rochester, NY, April 11, 2008, "Investigating student application of mathematical concepts in thermal physics," J.R. Thompson

Contributed presentations (12 oral, 18 poster, through April 2008)

- Joint American Physical Society / American Association of Physics Teachers (APS/AAPT) Regional Meeting, New England Section, MIT, Cambridge, MA, April 2005:

  "Investigating student understanding of entropy and the Second Law of Thermodynamics," with **B.R. Bucy** and D.B. Mountcastle.

  "Assessing Student Mathematical Preparation for Thermal Physics," with **D.B. Mountcastle** and B.R. Bucy. (Poster.)
- 2005 Summer *National* AAPT Meeting, U. of Utah, Salt Lake City, UT, August 2005:

  "Learning entropy and the Second Law of Thermodynamics as juniors," with **B.R. Bucy** and D.B. Mountcastle.

  "Identifying student difficulties with partial derivatives in thermodynamics," with B.R. Bucy and D.B. Mountcastle.
- 2005 Physics Education Research Conference, U. of Utah, Salt Lake City, UT, August 2005:

  "What is entropy? Assessing advanced undergraduate performance comparing ideal gas processes," with **B.R. Bucy** and D.B. Mountcastle. (Poster.)

  "Student understanding of partial differentiation in thermal physics," with B.R. Bucy and D.B. Mountcastle. (Poster.)
- *Foundations and Frontiers in Physics Education Research*, College of the Atlantic, Bar Harbor, ME, August 2005:

  "What is entropy? Assessing advanced undergraduate performance comparing ideal gas processes," with B.R. Bucy and **D.B. Mountcastle.** (Poster.)

  "Student understanding of partial differentiation in thermal physics," with B.R. Bucy and D.B. Mountcastle. (Poster.)
- 2006 Winter *National* AAPT Meeting, Anchorage, AK, January 2006, "Uneven Development of Students' Reasoning Regarding Concepts in Thermal Physics," with **D. Meltzer** (U. Washington) and W.M. Christensen (Iowa St. U.).
- Joint Meeting of the New England Sections of the AAPT and APS (regional), Boston University, Boston, MA, March/April 2006:

  "Student (mis)application of partial differentiation to material properties," with **B.R. Bucy** and D.B. Mountcastle.

  "Student understanding of differentials and the Maxwell relations in thermodynamics," with B.R. Bucy and D.B. Mountcastle. (Poster.)

- *Integrating Science and Mathematics Education Research into Teaching,* The University of Maine, Orono, ME, June 2006:

  "Student Estimates of Probability and Uncertainty in Statistical Physics," with **D.B. Mountcastle** and B.R. Bucy. (Poster.)

  "Student (mis)application of partial differentiation to material properties," with **B.R. Bucy** and D.B. Mountcastle. (Poster.)

- 2006 Summer National Meeting of the American Association of Physics Teachers (AAPT), Syracuse U., Syracuse, NY, July 2006:

  Student use of integration in the context of P-V diagrams," B.R. Bucy, J.R. Thompson, and D.B. Mountcastle.

  "Student (mis)application of partial differentiation to material properties," B.R. Bucy, J.R. Thompson, and D.B. Mountcastle. (Poster)

- 2006 Physics Education Research Conference, Syracuse U., Syracuse, NY, July 2006:

  "Student (mis)application of partial differentiation to material properties," B.R. Bucy, J.R. Thompson, and D.B. Mountcastle. (Poster)

  "Student estimates of probability and uncertainty in statistical physics," D.B. Mountcastle and B.R. Bucy, and J.R. Thompson. (Poster)

- 19th Biennial Conference on Chemical Education, Purdue U., West Lafayette, IN, August 2006, "Investigating Upper-Division Student Understanding of Thermal Physics."
- 2007 Winter National Meeting of the AAPT, Seattle, WA, January 2007, "Student Estimates of Probability and Uncertainty in Statistical Physics," D.B. Mountcastle, B.R. Bucy, and John R. Thompson. (Poster)
- 2007 March APS Meeting, Denver, CO, March, 2007, "Student application of integration when considering *P-V* diagrams," J.R. Thompson, B.R. Bucy, D.B. Mountcastle, E.B. Pollock.
- Joint Meeting of the New England Sections of the AAPT and APS, University of Maine, Orono, ME, April 2007:

  "Comparing student understanding of physics and mathematics in *P-V* diagrams," E.B. Pollock, J.R. Thompson, B.R. Bucy, D.B. Mountcastle. (Poster)

  "Student Estimates of Probability and Uncertainty in Advanced Laboratory and Statistical Physics Courses," D.B. Mountcastle, B.R. Bucy, and J.R. Thompson. (Poster)

- University of Maine Graduate Student Government Research Exposition, Orono, ME, April 2007, "Comparing student understanding of physics and mathematics in *P-V* diagrams," E.B. Pollock, J.R. Thompson, B.R. Bucy, D.B. Mountcastle. (Poster)
- 2007 Summer National Meeting of the American Association of Physics Teachers (AAPT), Greensboro, NC, July 2007:

  "Interpretations of entropy among advanced undergraduates across disciplines," B.R. Bucy, J.R. Thompson, and D.B. Mountcastle

“Investigating mathematical fluency among upper-division physics students,” D.B. Mountcastle, B.R. Bucy, and J.R. Thompson

“Comparing advanced undergraduate reasoning about entropy across disciplines,” B.R. Bucy, J.R. Thompson, and D.B. Mountcastle (Poster)

“Comparing student understanding of physics and mathematics in P-V diagrams,” E.B. Pollock, J.R. Thompson, B.R. Bucy, and D.B. Mountcastle (Poster)

“Student estimates of probability and uncertainty in advanced laboratory and statistical physics courses,” D.B. Mountcastle, B.R. Bucy, and J.R. Thompson. (Poster)

presentations given after the grant period, but based on work done during the grant duration

- 2008 American Physical Society April Meeting, St. Louis, MO, April 2008:

  “Investigating student understanding of partial differentiation in upper-level thermodynamics I: Identifying student difficulties,” J.R. Thompson, B.R. Bucy, and D.B. Mountcastle

  “Investigating student understanding with partial differentiation in thermodynamics II: Development and assessment of curriculum,” B.R. Bucy, J.R. Thompson, and D.B. Mountcastle

Publications

Peer-reviewed conference proceedings (5):

D.B. Mountcastle, B.R. Bucy, and J.R. Thompson, “Student estimates of probability and uncertainty in advanced laboratory and statistical physics courses,” in *2007 Physics Education Research Conference,* L. Hsu, C. Henderson, L. McCullough, eds., AIP Conference Proceedings **951**, 152-155 (2007).

E.B. Pollock, J.R. Thompson, and D.B. Mountcastle, “Student understanding of the physics and mathematics of process variables in P-V diagrams,” in *2007 Phys. Educ. Res. Conf.,* L. Hsu, C. Henderson, L. McCullough, eds., AIP Conference Proceedings **951**, 168-171 (2007).

B.R. Bucy, J.R. Thompson, and D.B. Mountcastle, “Student (Mis)application of Partial Differentiation to Material Properties,” in *2006 Phys. Educ. Res. Conf.,* L. McCullough, L. Hsu, P. Heron, Eds., AIP Conference Proceedings **883**, 157-160 (2007).

J.R. Thompson, B.R. Bucy, and D.B. Mountcastle, “Assessing student understanding of partial derivatives in thermodynamics,” in *2005 Phys. Educ. Res. Conf.,* P. Heron, L. McCullough, J. Marx, Eds., AIP Conference Proceedings **818**, 77-80 (2006).

B.R. Bucy, J.R. Thompson, and D.B. Mountcastle, “What is entropy? Advanced undergraduate performance comparing ideal gas processes,” in *2005 Phys. Educ. Res. Conf.,* P. Heron, L. McCullough, J. Marx, Eds., AIP Conference Proceedings **818**, 81-84 (2006).

Manuscripts in preparation (2 active, 2-3 in the queue):

B.R. Bucy, J.R. Thompson, and D.B. Mountcastle, “Student understanding of entropy and entropy changes in the context of ideal gas processes,” manuscript in preparation for submission to the *American Journal of Physics*.

B.R. Bucy, J.R. Thompson, and D.B. Mountcastle, "Student understanding of the equality of mixed second-order partial derivatives in the context of thermodynamics," manuscript in preparation for submission to the *American Journal of Physics*.

- We anticipate several submissions to journals in physics education and physics education research (e.g., *Physical Review Special Topics – Physics Education Research* and the *American Journal of Physics*), as well as a more general article about the cross-disciplinary work to a science education research journal (e.g., *J. Res. Sci. Teach.*).
- We are also working with our collaborators (Meltzer and Christensen) to prepare a manuscript comparing the results on different questions about entropy and the second law to give a multi-context picture of student understanding across multiple questions, with different representations, and the implications for the effectiveness of specific contexts and representation on student understanding and learning.

Dissertations and Theses (1 Ph.D. dissertation completed, 1 M.S. thesis expected)

Brandon R. Bucy, "Investigations of Student Understanding of Entropy and of Mixed Second-Order Partial Derivatives in Upper-Level Thermodynamics." Ph.D. (Physics), August 2007.

Evan B. Pollock, "Investigations of Student Understanding of the mathematics and physics of *P-V* Diagrams." M.S. (Physics), anticipated August 2008.