

PHY 770 -- Statistical Mechanics
10-10:50 AM MWF Olin 107

Instructor: Natalie Holzwarth (Olin 300)
 Course Webpage: <http://www.wfu.edu/~natalie/s14phy770>

A Modern Course in Statistical Physics
 Third Revised and Updated Edition

<http://www.wiley.com/WileyCDA/WileyTitle/productCd-3527407820.html>

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Textbook Chapters	Course topics
1. Introduction	
2. Complexity and entropy	3
3. Thermodynamics	1
4. Thermodynamics of phase transitions	2
5. Equilibrium Statistical Mechanics I	4
6. Equilibrium Statistical Mechanics II	5
7. Brownian Motion	6
8. Hydrodynamics	7
9. Transport coefficients	8
10. Nonequilibrium phase transitions	9

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PHY 770 Statistical Mechanics

TR 12:30-1:45 PM OPL 107 <http://www.wfu.edu/~natalie/s14phy770/>

Instructor: [Natalie Holzwarth](#) Phone: 758-5510 Office: 300 OPL e-mail: natalie@wfu.edu

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- [Lecture notes](#)

Last modified: Monday, 13-Jan-2014 21:49:50 EST

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General Information

This course is a one semester survey of Statistical Mechanics at the graduate level, using the textbook: *A Modern Course in Statistical Physics*, 3rd edition, by Linda E. Reichl (Wiley-VCH, 2009).

It is likely that your grade for the course will depend upon the following factors:

Problem sets*	45%
Presentation	10%
Exams	45%

*The schedule notes the "due" date for each assignment. Homeworks may be turned in 1 lecture past their due date without grade penalty. After that, the homework grade will be reduced by 10% for each succeeding late date. According to the honor system, all work submitted for grading purposes should represent the student's own best efforts. This means that students who work together on homework assignments should all contribute roughly equally and independently verify all derivations and results.

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Course schedule for Spring 2014

(Preliminary schedule -- subject to frequent adjustment.) Please note that makeup lectures (indicated in red) are scheduled for Tuesdays or Thursdays at 11 AM - 12:15 PM in Olin 107.

Lecture date	Text Reading	Topic	Assign.	Due date
1 Tue: 01/14/2014	Chap. 3	Review of macroscopic thermodynamics	#1	02/04/2014
2 Thu: 01/16/2014	Chap. 3	Review of macroscopic thermodynamics	#2	02/04/2014
3 Tue: 01/21/2014	Chap. 3			02/04/2014
4 Tue: 01/21/2014	Chap. 3			02/04/2014
5 Thu: 01/23/2014	Chap. 3			02/04/2014
Tue: 01/28/2014		NAWH out of town - no class.		
Thu: 01/30/2014		NAWH out of town - no class.		
6 Tue: 02/04/2014	Chap. 3			02/06/2014

PHY 770 -- Assignment #1

January 14, 2014

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Spring 2014 Schedule for N. A. W. Holzworth

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00-10:00	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours	Lecture Preparation/ Office Hours
10:00-11:00	Electrodynamics PHY712	Office Hours	Electrodynamics PHY712	Office Hours	Electrodynamics PHY712
11:00-12:30	Office Hours	Makeup Lectures PHY712/770	Office Hours	Makeup Lectures PHY712/770	Office Hours
12:30-2:00	Condensed Matter Theory Journal Club	Condensed Matter Theory Journal Club	Physics Research	Condensed Matter Theory Journal Club	Physics Research
2:00-3:30	Condensed Matter Monthly Meeting	Physics Research	Physics Research	Physics Research	Physics Research
3:30-5:00	Physics Research	Physics Research	Physics Colloquium	Physics Research	Physics Research

Travel dates:

- Jan. 27 - Jan. 30, 2014 – CGCAM meeting on "Pseudopotentials and PAW atomic data: beyond a "black art"?" in Paris, France
- Feb. 24 - Feb. 28, 2014 – 27th Annual Workshop on "Recent Developments in Computer Simulations Studies in Condensed Matter Physics" in Athens, GA.
- Mar. 5 - 7 -- March 2014 APS Meeting in Denver, CO.

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Today's topics – review of thermodynamics (Chapter 3 of text)

1. Overview and motivation
2. Important definitions
3. Meaning of thermodynamic equilibrium
4. Notion of exact differential and its opposite
5. State variables
6. First law of thermodynamics
7. Carnot cycle
8. Notion of entropy

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Thermodynamics

1. Overview and motivation

Some ideas from **Advanced Statistical Mechanics**, Barry M. McCoy (2010)

- The development of the notions of thermodynamics occurred in the 19th century with its results at the “heart of the industrial revolution”.
- Notions of thermodynamics do not logically follow from Newton’s laws. (Within Statistical Mechanics, connections between the macroscopic thermodynamic principles and the microscopic viewpoint of Newton’s laws are explored.
- “We are forced to study thermodynamics because nature empirically turns out to work this way. Because thermodynamic behavior exists it must follow from the microscopic laws of nature, regardless of how much we may not like it.”

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Thermodynamics

2. Important definitions

Macroscopic system, "thermodynamic limit"
 For a system of N particles in a volume V :

$N \rightarrow \infty$ and $V \rightarrow \infty$ with

$$\frac{N}{V} \equiv \nu = \frac{1}{\rho} \text{ fixed}$$

Intensive variable: (such as T, P, μ, \dots)
 (intensive) $_{N \rightarrow \infty} = \text{constant}$

Extensive variable: (such as $N \dots$)
 (extensive/ N) $_{N \rightarrow \infty} = \text{constant}$

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Thermodynamics

3. Notion of thermodynamic equilibrium

We observe that the properties of an isolated macroscopic system measured as a function of time, eventually reach constant values. (This is not true, in general, for a system of few particles.)

3. This problem concerns heat transfer between various materials placed within a thermally isolated container. You may use the information given in the following table:

Specific heat of ice at $T \leq 0^\circ\text{C}$	2090 J/(kg $^\circ\text{C}$)
Specific heat of water for $0^\circ\text{C} \leq T \leq 100^\circ\text{C}$	4186 J/(kg $^\circ\text{C}$)
Latent heat of fusion for water at $T=0^\circ\text{C}$	333000 J
Latent heat of vaporization for water at $T=100^\circ\text{C}$	2260000 J

a. Initially, the container contains the following

- 0.7 kg of water at 100°C
- 0.2 kg of ice at -0.5°C

When the system comes to equilibrium, is there any ice left in the system? What is the temperature of the system when it comes to equilibrium?

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When the system comes to equilibrium, is there any ice left in the system? What is the temperature of the system when it comes to equilibrium?

Solution

a. Assume all ice melts, keep temperature in Celsius

$$Q = 0 + 0.7 \cdot 4186 \cdot (T_f - 100) + 0.2 \cdot 2090 \cdot (0 + 0.5) + 0.2 \cdot 333000 + 0.2 \cdot 4186 \cdot (T_f - 0)$$

$$T_f = 60.04^\circ\text{C}$$

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Thermodynamics
 4. Notion of exact differential and its opposite

A function $F(x, y)$ has an exact differential dF iff :

$$dF = \left(\frac{\partial F}{\partial x}\right)_y dx + \left(\frac{\partial F}{\partial y}\right)_x dy$$

with

$$\left(\frac{\partial}{\partial y}\left(\frac{\partial F}{\partial x}\right)_y\right)_x = \left(\frac{\partial}{\partial x}\left(\frac{\partial F}{\partial y}\right)_x\right)_y$$

An inexact differential is denoted dF

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Example (from appendix B.1 of textbook)

Consider : $dF = (x^2 + y)dx + (x)dy$

By integrating, can show that :

$$F(x, y) = \frac{1}{3}x^3 + xy + C$$

Note that this implies

$$\int_A^B dF = F(x_B, y_B) - F(x_A, y_A)$$

Example of inexact differentials :

Heat added to system : dQ

Work done by system : dW

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Thermodynamics
 5. State variables

State variables are quantities that can be analyzed as exact differentials

Examples :
 (Under *reversible* conditions)
 Internal energy U
 Entropy S

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Thermodynamics
 6. First law of thermodynamics

Notation :

- Differential internal energy : dU
- Heat added to system : dQ
- Work done by system : dW
- Differential particles of type j : dN_j
- Chemical potential of type j particles : μ_j

$$dU = dQ - dW + \sum_{j=1}^N \mu_j dN_j$$

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Elaboration on work:

$$dW = PdV - JdL - \alpha dA - \mathbf{E} \cdot d\mathbf{P} - \mathbf{H} \cdot d\mathbf{M} - \Phi dq$$

$$\equiv -YdX$$

Specific example:
 Consider an ideal gas in a complete cycle

$$PV = NkT \quad (k \equiv k_B \text{ Boltzmann constant})$$

$$U = \frac{k}{\gamma - 1} NT = \frac{PV}{\gamma - 1} \quad (\gamma = C_p / C_v)$$

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Carnot cycle:
 Analysis of an ideal heat engine
 Nicholas Carnot (French Engineer) 1834

Figure 2.9: The four steps of the Carnot cycle.

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Analysis of Carnot cycle for ideal gas system

$$U_{12} = 0 \Rightarrow Q_{12} = W_{12} = NkT_{high} \ln \frac{V_2}{V_1}$$

$$Q_{23} = 0 \Rightarrow U_{23} = -W_{23} = \frac{Nk(T_{low} - T_{high})}{\gamma - 1}$$

$$U_{34} = 0 \Rightarrow Q_{34} = W_{34} = NkT_{low} \ln \frac{V_4}{V_3}$$

$$Q_{41} = 0 \Rightarrow U_{41} = -W_{41} = \frac{Nk(T_{high} - T_{low})}{\gamma - 1}$$

$$\eta = \frac{W_{total}}{Q_{input}} = \frac{W_{12} + W_{34}}{Q_{12}}$$

$$= 1 + \frac{NkT_{low} \ln(V_4/V_3)}{NkT_{high} \ln(V_2/V_1)}$$

$$= 1 - \frac{T_{low}}{T_{high}}$$

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More analysis of Carnot cycle for ideal gas system

$$\eta = \frac{W_{total}}{Q_{input}} = \frac{W_{12} + W_{34}}{Q_{12}} = \frac{Q_{12} + Q_{34}}{Q_{12}}$$

$$= \frac{|Q_{high}| - |Q_{low}|}{|Q_{high}|} = 1 - \frac{T_{low}}{T_{high}}$$

$$\frac{|Q_{low}|}{|Q_{high}|} = \frac{T_{low}}{T_{high}} \Rightarrow \frac{|Q_{low}|}{T_{low}} = \frac{|Q_{high}|}{T_{high}}$$

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Definition of entropy for a reversible process:

$$dS = \frac{dQ}{T}$$

Example for Carnot cycle:

$$S_{12} = \frac{Q_{12}}{T_{high}} = \frac{Q_{high}}{T_{high}} = Nk \ln \frac{V_2}{V_1}$$

$$Q_{23} = 0 \Rightarrow S_{23} = 0$$

$$S_{34} = \frac{Q_{34}}{T_{low}} = \frac{-|Q_{low}|}{T_{low}} = Nk \ln \frac{V_4}{V_3}$$

$$Q_{41} = 0 \Rightarrow S_{41} = 0$$

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Analysis of state variables U and S for an ideal gas

$$dS = \frac{dQ}{T} \quad dW = PdV \quad dU = TdS - PdV$$

For ideal gas: $PV = NkT$

$$U = \frac{Nk}{\gamma-1} T = \frac{PV}{\gamma-1} \quad (\gamma = C_p / C_v)$$

If N is constant: $dU = \frac{Nk}{\gamma-1} dT = TdS - PdV$

$$\text{For } S = S(T, V): \quad dS = \frac{Nk}{\gamma-1} \frac{1}{T} dT + \frac{Nk}{V} dV$$

$$\begin{aligned} \Rightarrow S(T, V) &= \frac{Nk}{\gamma-1} (\ln(T) + \ln(V^{\gamma-1})) + (\text{constant}) \\ &= \frac{Nk}{\gamma-1} \left(\ln \left(\frac{TV^{\gamma-1}}{T_0 V_0^{\gamma-1}} \right) \right) + (\text{constant}) \end{aligned}$$

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Analysis of ideal gas entropy continued:

For ideal gas: $PV = NkT$

$$U = \frac{Nk}{\gamma-1} T = \frac{PV}{\gamma-1}$$

If N is constant: $dU = \frac{Nk}{\gamma-1} dT = TdS - PdV$

$$S(T, V) = \frac{Nk}{\gamma-1} \left(\ln \left(\frac{TV^{\gamma-1}}{T_0 V_0^{\gamma-1}} \right) \right) + (\text{constant})$$

Check with Exercise 3.2 of textbook: (with $\gamma = 5/3$)

$$S = \frac{5}{2} Nk + Nk \ln \left(\frac{T^{5/2}}{P} \right) + Nk \ln \left(\left(\frac{2\pi m}{h^2} \right)^{3/2} k^{5/2} \right)$$

Note: $\ln \left(\frac{T^{5/2}}{P} \right) = \frac{1}{2/3} \ln(T^{2/3}) + (\text{constant})$ quantum effects;
consistent with "constant"

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Analysis of ideal gas entropy and internal energy continued:

For ideal gas: $U = \frac{Nk}{\gamma-1} T$

$$S(T, V) = \frac{Nk}{\gamma-1} \left(\ln \left(\frac{TV^{\gamma-1}}{T_0 V_0^{\gamma-1}} \right) \right) + S_0$$

$$\Rightarrow T = \frac{T_1}{(V/V_1)^{\gamma-1}} \exp \left(\frac{\gamma-1}{Nk} (S - S_0) \right)$$

$$\Rightarrow U(S, V) = \frac{Nk}{\gamma-1} \frac{T_1}{(V/V_1)^{\gamma-1}} \exp \left(\frac{\gamma-1}{Nk} (S - S_0) \right)$$

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