# Preface

The purpose of writing this book is to explain basic concepts of equilibrium statistical mechanics to the first year graduate students in engineering departments. Why should an engineer care about statistical mechanics?

Historically, statistical mechanics evolved out of the desire to explain thermodynamics from fundamental laws of physics governing behavior of atoms and molecules. *If* a microscopic interpretation of the laws of thermodynamics were the only outcome of this branch of science, statistical mechanics would not appeal to those of us who simply wish to use thermodynamics to perform practical calculations. After all, validity of thermodynamics has long been established.

In thermodynamics, a concept of fundamental equations plays a prominent role. From one such equation many profound predictions follow in a completely general fashion. However, thermodynamics itself does *not* predict the explicit form of this function. Instead, the fundamental equation must be determined empirically for each system of our interest. Being a science built on a set of macroscopic observations, thermodynamics does not offer any systematic way of incorporating molecular level information, either. Thus, an approach based solely on thermodynamics is not sufficient if we hope to achieve desired materials properties through manipulation of nanoscale features and/or molecular level architecture of materials.

It is in this context that the method of statistical mechanics becomes important for us. Equilibrium statistical mechanics provides a general framework for constructing the fundamental equation from a molecular level description of the system of interest. It can also provide a wealth of molecular level insights that is otherwise inaccessible even experimentally. As such, it is becoming increasingly more relevant to engineering problems, requiring majority of engineering students to develop more than just a passing acquaintance with the basic results of this subject.

Because statistical mechanics is built on the basis of classical and quantum mechanics, some elementary knowledge of these subjects proves essential in order to access the existing textbooks on statistical mechanics in any meaningful manner. However, these subjects fall outside the expected background of engineering students. For some, these subjects are entirely foreign. This book is meant to fill in the gap felt by such students, who need to efficiently absorb only those essential back-

grounds necessary to understand the basic ideas of statistical mechanics and quickly move onto more specific topics of their own interest.

My intention, therefore, is not to replace many excellent textbooks on statistical mechanics that exist today, but *to ease the transition* into such textbooks. Thus, I did not try to showcase various applications of statistical mechanics, of which there are many. Instead, the emphasis is on making the basic ideas of statistical mechanics accessible to the intended audience. The end result is this book, serving as a gentle introduction to the subject. By the end of this book, however, you will be well positioned to read more advanced textbooks including those with more specialized themes, some of which are listed in Appendix E.

In this book, I have chosen to present classical mechanical formulation of statistical mechanics. This is somewhat contrary to the prevailing wisdom that favors the mathematical simplicity of quantum statistical mechanics: Microstates in quantum mechanical systems can be counted, at least in principle. This is not so in classical mechanical systems *even in principle*. However, relevant concepts in quantum mechanics are far more abstract than those in classical mechanics and a proper understanding of the former requires that of the latter. A common compromise is to simply accept the discrete energy spectrum of bound quantum states. But, this leaves a rather uncomfortable gap in the students' knowledge. No less important is the fact that many applications of statistical mechanics in engineering problems take place within essentially the classical framework even though the fundamental laws of physics dictating the behavior of atoms are quantum mechanical in nature.

It seemed inappropriate to use a symbol that is either very different from established conventions or far detached from the meaning it is supposed to represent. The alternative has an unfortunate consequence that multiple meanings had to be given to a single symbol on occasion. In such cases, the context should always dictate what is meant by the particular symbol in question. In this regard, notation is no different from an ordinary language. To minimize a possible confusion, a list of frequently used symbols is provided at the end of each chapter.

## Suggestions Before You Start

A prior exposure to undergraduate level thermodynamics will be very helpful as it provides you with a sense of direction throughout our journey ahead. I will also assume that you have a working knowledge of calculus. Specifically, you should know how to evaluate derivatives and integrals of functions of multiple variables. In case you need to regain some of these skills, I tried to include as much calculational details as reasonable. However, calculus is a perishable skill and a constant practice is essential in maintaining a certain level of proficiency. More importantly, "Mathematics is a language in which the physical world speaks to us."[1] That is, you cannot expect to understand the subject without penetrating through certain manipulative aspects first. I made no attempt to conceal this fact. It is up to you to fill in the missing steps of the calculations with a stack of papers and a pencil on your side.

Though this will *not* change the content of any given equation, it will profoundly change your relationship to that equation.

To help you learn new concepts, exercises are scattered throughout the book. Keeping with the above stated goal of this book, most of them require only a fairly straightforward (I hope) manipulation of equations and applications of concepts just learned. The primary reward for solving these problems is *not* the final answer per se but the *perspective you gain from working through them*. You are strongly urged to attempt as many of them as possible. So that the exercises will not become an undue hindrance to your progress, hints are given to a subset of them in Appendix G.

The materials covered in Chap. 1 through Chap. 5 form the core of this book and should be sufficient if you want to transition to more advanced textbooks as quickly as possible. Chapters 6 and 7 are concerned with thermodynamics and statistical mechanics of inhomogeneous fluids. So that you would not have to feel uncomfortable when consulting existing textbooks on statistical mechanics, Chap. 8 introduces key concepts from quantum mechanics and briefly illustrates their application in formulating statistical mechanics.

In the main body of the book, you will notice that some section headings bear a dagger (†). These sections are aimed at exploring issues prompted by questions from students in my graduate level courses on thermodynamics and statistical mechanics. Some of them provide detailed derivations of key results that are simply quoted in undaggered sections. Sections marked with double dagger (‡) cover materials that are considered standard by many, including myself. But, they can be brushed aside in view of our immediate goal. These optional sections were retained in the hope that they may spice up your journey through the book. Some are retained as a modest attempt at completeness. If you are pressed for time, or simply do not want to bother with them at this time, you can omit them without any guilt or loss of continuity until your curiosity compels you otherwise. On occasion, I do use certain results from these optional sections, but only with an explicit reference to the relevant sections. You can either choose to read the indicated section at that time, or simply accept the results quoted and move on. After all, learning is an iterative process and there is no need to absorb everything in your first attempt at the subject. Enjoy!

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Isamu Kusaka
kusaka.2@osu.edu

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