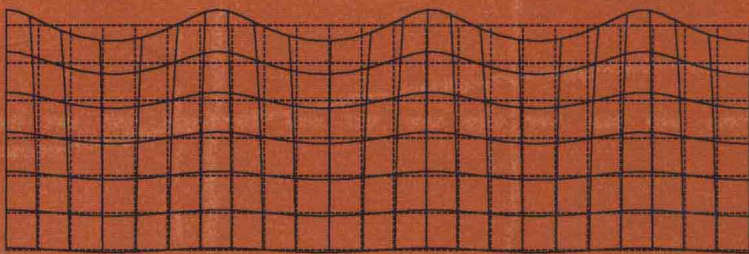


Andrew N. Cleland

Foundations of Nanomechanics

From Solid-State Theory
to Device Applications



Springer

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Preface

Why write another book on mechanics? There are, after all, a number of excellent texts that describe in great detail the way classical solids behave when acted upon by static and time-varying forces; many of these are cited in this monograph. These texts treat solids as continuous objects, and quantum mechanics does not enter the discussion. Furthermore, the atomic nature of the solid is implicit, but does not enter in a central role. At the other end of the spectrum, texts on condensed matter physics focus on the quantum mechanical nature of the solid; these contain quite clear descriptions of acoustic waves in solids, describing their dynamic and thermal properties, and how they interact with electrons in the solid, but contain little information regarding bulk deformations.

This text, focussing on the mechanics of very small objects, attempts to provide a link between these two approaches; in addition to describing the theories of both the classical and the quantum mechanical solid, I attempt to outline where the classical description breaks down, and quantum mechanics must be applied, to understand the behavior of a nanoscale object. I have tried to merge the continuum description of the solid with the atomic one, and to show how and where quantum mechanics plays a role, especially as the size scale of the system is reduced, making the quantized energy scale *larger* and the role of thermal vibrations more important.

This text is designed to be an introduction for physicists and engineers to the basic foundations of solid mechanics, treating both the static and dynamic theories. We begin with a simplified atomistic description of solids, starting in Chap. 1 with the problem of two atoms in a bound state and then extending the discussion to three and then N atoms in a linear chain. In Chap. 2 we cover the microscopic description of the mechanics of three dimensional insulating solids, from the same basic condensed matter viewpoint, and in Chap. 3 touch on the thermal and transport properties for phonons, the quantized mechanical excitations of a solid. In Chaps. 4–7 we connect the microscopic description to the conventional description of continuum dynamics, introducing the concepts of strain and stress, their interplay and their control of the mechanical function of deformable solids, and then dealing with both static and dynamic problems in continuum mechanics. In Chap. 8 we touch on the topic of dissipation and noise in mechanical systems.

In the last three chapters, Chaps 9–11, we describe a number of experimental implementations of nanomechanical devices, and also give an outline of the techniques involved in patterning and fabricating nanomechanical structures

This text is written at an advanced undergraduate or beginning graduate student level. It should also prove useful for the practicing engineer or scientist. The reader is expected to have a good grounding in classical, rigid-body mechanics, covered in most first-year courses. An understanding of vector calculus and linear algebra is assumed, so that the reader should be familiar with divergence and gradient operators, as well as how to invert and diagonalize a matrix, and take a determinant. No background in solid mechanics is assumed, nor is any knowledge of semiconductor processing, the main tool for the fabrication of nanometer-scale devices. Exercises are provided at the end of each chapter, and range in difficulty as the exercise number goes up.

Some notes on symbols. I have chosen to use bold, italic roman symbols for vectors such as \mathbf{u} , and bold, sans-serif symbols for tensors such as \mathbf{R} . Scalars are written in italic roman type as in G , and components of vector or tensors written as italic roman with roman subscripts such as R_{ij} . A list of commonly used symbols, and their units and conversion in the Système Internationale (SI) and centimeter-gram-second (CGS) systems appears at the end of the book.

I would like to express my appreciation to those who read and commented on sections of the unfinished manuscript, including Dr. Robert Knobel, Derek Barge, and Kang-kuen Ni. I would also like to express my thanks to my wife Ning and my children Agnetta and Nicholas for their patience while I was working on this book.

Santa Barbara and Los Angeles
July, 2002

Andrew N. Cleland

Contents

1. Introduction: Linear Atomic Chains	1
1.1 A Model Binary Molecule: Two Atoms	1
1.1.1 External Forces	4
1.1.2 Dynamic Motion	6
1.2 The Three Atom Chain	8
1.2.1 External Force on a Trimer	9
1.2.2 Strain in the Trimer	10
1.2.3 Dynamic Motion	10
1.3 An N -mer Molecule: The N Atom Linear Chain	13
1.3.1 Normal Mode Coordinates	17
1.3.2 Phase and Group Velocity	19
1.3.3 Fixed Boundary Conditions	20
1.3.4 Transverse Motion	22
1.4 Linear Chain with Optical Modes	26
1.5 Quantum Mechanics and Thermodynamics of the Linear Chain	29
1.6 Effect of Temperature on the Linear Chain	30
1.6.1 Specific Heat for an N Atom Chain	33
1.6.2 Thermal Expansion	35
1.7 Quantum Operators for Normal Modes	37
1.7.1 Quantum Operators for the Simple Harmonic Oscillator	37
1.7.2 Quantum Operators for the N -Atom Chain	39
Exercises	40
2. Two- and Three-Dimensional Lattices	43
2.1 Crystal Lattices	43
2.2 Two-Dimensional Crystals	44
2.3 Three-Dimensional Crystals	46
2.3.1 Crystal Structures with a Basis	48
2.4 Periodic Functions	49
2.4.1 One-Dimensional Fourier Series	50

2.4.2	Two and Three Dimensional Fourier Series: The Reciprocal Lattice	51
2.4.3	Reciprocal Space Lattices: Some Examples	53
2.5	Bloch's Theorem	54
2.6	Classical Theory of the Lattice	56
2.6.1	Diatomic Interaction Potentials	59
2.6.2	Boundary Conditions in Two and Three Dimensions ..	62
2.6.3	Normal Modes of the Lattice.....	63
2.6.4	Optical Phonons	75
2.7	Normal Mode Hamiltonian	75
2.7.1	Quantum Operators for Normal Modes.....	77
2.8	Connection to the Classical Continuum Theory of Solids.....	79
	Exercises	84
3.	Properties of the Phonon Gas	87
3.1	Specific Heat of the Phonon Gas	87
3.1.1	Primary Thermal Phonon Wavelength	95
3.2	Phonons as Particles: Position, Momentum and Scattering	100
3.2.1	Phonon Momentum and Energy	102
3.3	Phonon Scattering from Point Defects.....	104
3.4	Phonon-Phonon Interactions.....	109
3.4.1	Phonon-Phonon Interactions: Temperature Dependence.....	114
3.4.2	Higher Order Phonon-Phonon Interactions.....	115
3.4.3	Akhiezer Effect	116
3.5	Electron-Phonon Scattering	119
3.5.1	Piezoelectric Interaction.....	127
3.6	Phonon Thermal Conductivity	131
3.6.1	The Boltzmann Equation.....	133
3.6.2	Quantum of Thermal Conductance	137
3.6.3	Thermal Conductivity in Metals.....	140
	Exercises	143
4.	Stress and Strain	145
4.1	Relative Displacement and Strain.....	145
4.2	Principal Axes of Strain	152
4.3	Superposition	155
4.3.1	Eulerian Definition of Strain	156
4.4	The Stress Tensor	157
4.4.1	Symmetry of the Stress Tensor	162
4.5	Properties of the Stress Tensor	162
4.5.1	Transformations of the Stress Tensor.....	162
4.5.2	Stress on an Arbitrary Surface	164
4.5.3	Principal Axes of Stress	165

4.6	Inhomogeneous Stresses and Arbitrary Shapes	167
4.7	Body Forces	168
4.7.1	Torque Balance in the Presence of Body Forces	170
	Exercises	172
5.	Elasticity Relations	175
5.1	Classes of Elastic Response	175
5.2	Linear Elastic Response	177
5.2.1	Six-Vector Representation of Stress and Strain	178
5.2.2	Elastic Stiffness	179
5.3	Orthotropic and Isotropic Materials	179
5.4	Crystalline Materials	184
5.5	Strain–Stress Relations	187
5.6	Polycrystalline Materials	188
5.7	Conclusion	189
	Exercises	189
6.	Static Deformations of Solids	191
6.1	System of Equations for a Static Deformable Solid	191
6.1.1	Boundary Conditions	193
6.2	Extensional Forces	194
6.2.1	Extension of a Beam from End Forces	195
6.2.2	Extension of a Beam from a Body Force	196
6.3	Flexure of Beams	198
6.3.1	Bending by Pure Torque	199
6.3.2	Displacement of the Neutral Axis	201
6.3.3	Saint–Venant’s Principle	202
6.4	Euler–Bernoulli Theory of Beams	203
6.4.1	Torque and Shear due to Local Forces	205
6.4.2	Shear Displacements	208
6.4.3	Boundary Conditions	209
6.4.4	Point Forces	210
6.4.5	Results for Common Bending Problems	210
6.5	Torsional Beam	211
6.5.1	Torsion of Non-Circular Cylinders	214
6.6	Two-Dimensional Problems	215
6.6.1	Plane Strain	215
6.6.2	Plane Stress	217
6.7	Three-Dimensional Problems	218
	Exercises	221
7.	Dynamical Behavior of Solids	223
7.1	Simple Vibrational Methods: Torsional Vibrations in Beams	223
7.1.1	Longitudinal Vibrations	224
7.1.2	Torsion of Cylinders	229

7.1.3	Stress and Strain in Longitudinal and Torsional Motion	231
7.1.4	Flexural Vibrations	233
7.2	Dynamical Equations of Motion in an Isotropic Solid	240
7.3	Waves in Infinite Isotropic Solids	242
7.3.1	Dilational and Rotational Waves	242
7.3.2	Scalar and Vector Potentials Φ and \mathbf{H}	244
7.3.3	Time-Dependent Body Forces	246
7.4	Waves in Infinite Crystalline Solids	249
7.4.1	Energy Flow and the Poynting Vector in Crystalline Solids	251
7.5	Waves in Semi-infinite Isotropic Solids	254
7.5.1	Waves Incident at Normal Incidence	256
7.5.2	Waves Incident at Arbitrary Angles	257
7.5.3	Rayleigh Waves	261
7.6	Waves in Plates	264
7.6.1	Shear Horizontal Waves in Plates	265
7.6.2	The General Problem of Waves in a Plate	267
7.7	Waves in Rods	271
7.7.1	Torsional Waves	272
7.7.2	Longitudinal Waves	273
7.7.3	Flexural Waves	273
7.8	Summary	274
	Exercises	275
8.	Dissipation and Noise in Mechanical Systems	277
8.1	Langevin Equation	278
8.1.1	Dissipation and Quality Factor	281
8.1.2	Attenuation	282
8.2	Zener's Model of an Anelastic Solid	282
8.2.1	Two-Level Systems	284
8.3	Thermoelastic Relaxation	285
8.4	Phonon-Phonon Interactions	288
8.4.1	Attenuation in Metals	290
8.5	Dissipation in Nanoscale Mechanical Resonators	292
8.5.1	Driven Damped Beams	293
8.5.2	Dissipation-Induced Amplitude Noise	295
8.5.3	Dissipation-Induced Phase Noise	296
8.5.4	Frequency Noise	299
8.5.5	Allan Variance	300
	Exercises	301

9. Experimental Nanostructures	303
9.1 A Simple Fabrication Sequence	303
9.2 Flexural Resonators	305
9.2.1 Radiofrequency Flexural Resonators	305
9.2.2 Nonlinear Resonators	312
9.2.3 Free-Free Resonators	319
9.3 Parametric Resonators: The Mathieu Oscillator	321
9.3.1 Optical Parametric Resonator	329
9.4 Mechanical Electrometer	331
9.5 Thermal Conductance in Nanostructures	334
9.6 Coupling of Electron Transport and Mechanical Motion	336
9.7 Magnetic Resonance Force Microscopy	340
10. Nanostructure Fabrication I	349
10.1 Materials	350
10.2 Lithographic Principles	350
10.2.1 Photolithography	351
10.2.2 Electron Beam Lithography	355
10.2.3 Focused Ion Beams	360
10.2.4 Scanned-Probe Techniques: AFM and STM	361
10.2.5 Imprint Lithography	362
10.2.6 Self-Assembled Monolayers	363
10.3 Dry Etching Techniques	364
10.3.1 Plasma Etching	364
10.3.2 Reactive Ion Etching	365
10.3.3 Reactive Gas Chemistries	367
10.3.4 Silicon and Silicate Reactive Ion Etching	367
10.3.5 GaAs and GaAlAs Reactive Ion Etching	369
10.3.6 RIE Etching of Metals	369
10.3.7 Masking of RIE Etching	369
10.3.8 Ion Beam Etching	370
10.3.9 End-Point Detection	372
10.4 Wet Etching Techniques	373
10.4.1 Silicon Etchants	375
10.5 Thin Film Deposition	379
10.5.1 Evaporation and Sputtering Deposition of Thin Films	379
10.5.2 Chemical Vapor Deposition	382
10.5.3 Silicon Doping	389
10.5.4 Ion Implantation	390
10.6 Tunnel Junction Fabrication: Suspended Resist Mask	391

11. Nanostructure Fabrication II 395

 11.1 Bulk Single Crystal Nanomachining 395

 11.1.1 Silicon Regrowth Structures 399

 11.2 Epitaxial Heterostructure Nanomachining 399

 11.2.1 SIMOX and SLICE Wafers 399

 11.3 Polycrystalline Nanomachining 402

 11.4 GaAs Heterostructure-Based Nanofabrication 404

 11.5 Critical Point Drying 405

A. Mathematical Tools 407

 A.1 Scalars, Vectors, Tensors 407

 A.1.1 Vectors 407

 A.1.2 Tensors 410

 A.2 Eigenvectors and Eigenvalues 412

 A.3 The Dirac Delta Function 414

B. Compatibility Relations for Stress and Strain 417

C. Notation 421

Bibliography 423

Index 431

1. Introduction: Linear Atomic Chains

This book is aimed at developing a coherent description of what we term “nanomechanics”, the mechanical behavior of nanometer-scale objects, that is, objects for which at least one dimension is significantly less than $1\text{ }\mu\text{m}$. We will not concern ourselves with rigid body dynamics, those related to the motion of an object’s center of mass, and the rotation of the object about its center of mass; these are quite well described in a large number of texts, for both the classical and quantum mechanical limits. Instead we will focus on the static and dynamic deformations of solid objects, both with and without external forces. The self-resonant vibrational modes determine some of the thermodynamic properties of solids, such as the heat capacity and thermal conductivity; we touch on this connection as well. In the smallest structures, quantum mechanics must be applied to the description of the motion.

In the first part of this text, we provide the formalism required to understand these aspects in a unified manner, and we present a number of simple examples showing how the small size scale can impact and alter the bulk properties. In the second part of the text, we describe some approaches to fabricating and measuring the properties of nanoscale objects, providing some examples of actual devices.

We begin this chapter by discussing a very simple mechanical problem, that of a molecule of two atoms bound together by their mutual interaction. We restrict the motion of the atoms to one dimension, along the line connecting the atoms, and consider the response to external forces, and then work out the molecule’s natural vibrational resonance frequency. Next we move to a similar problem with three atoms, and then to the more general problem of the N atom chain. Following this heuristic discussion, we enter into a discussion of the quantum mechanical description of these systems, and conclude with the theory for the thermodynamic properties of the N atom chain.

1.1 A Model Binary Molecule: Two Atoms

Consider a molecule consisting of just two atoms. We restrict the motion of the two atoms to one dimension, along the line connecting them, so the atoms can only move directly towards or away from one another. We assume

that there is a net attractive force between the atoms; this may be due to an electrostatic attraction, if the atoms have opposite electric charges, to a chemical covalent bonding, where the outermost electrons are shared between the atoms, or to an attraction known as the *van der Waals* force, generated dynamically by the mutually induced dipole moments in each atom. At any rate, we assume that there is a force $f(r)$ between the two atoms, that depends only on the distance r between them. If this force is purely attractive, the atoms will accelerate and merge with one another. This however does not occur, because when the atoms get too close to one another, the electrons surrounding each atomic nucleus repel one another through their electrostatic interaction, and are furthermore limited by a fundamental law of quantum mechanics from occupying the same volume of space. The attractive force therefore becomes repulsive when the atoms get very close to one another.

As we shall see, it is often more useful to deal with the interaction potential energy $\phi(r)$ rather than the force $f(r)$, which is defined through the relation

$$f(r) \equiv -\frac{d\phi}{dr}. \quad (1.1)$$

Note that this differential equation defines the potential energy only up to an additive constant, whose value is arbitrary and has no physical meaning. The potential energy can also be described as the negative of the work done by the force for a displacement $r - r_0$ from the point of zero potential energy r_0 , or

$$\phi(r) = -W = -\int_{r_0}^r f(r) dr, \quad (1.2)$$

which is equivalent to (1.1).

As a specific example, we will consider the model known as the *Lennard-Jones* interaction, which applies to atoms interacting through the van der Waals interaction. The interaction potential energy for the Lennard-Jones model has the algebraic form

$$\phi(r) = -\frac{A}{r^6} + \frac{B}{r^{12}}, \quad (1.3)$$

with the parameter A determining the strength of the attractive interaction, and B the repulsive interaction. The attractive $1/r^6$ dependence is characteristic of the van der Waals interaction, while the repulsive $1/r^{12}$ dependence is somewhat phenomenological. The repulsive interaction is strongest for small r , with the atoms close together, and decreases more rapidly with r than the attractive interaction, which therefore dominates for large r . The zero for the potential energy $\phi(r)$ is chosen so that the energy is zero when the atoms are infinitely far apart. The force corresponding to (1.3) is

$$f(r) = 6 \frac{A}{r^7} - 12 \frac{B}{r^{13}}. \quad (1.4)$$

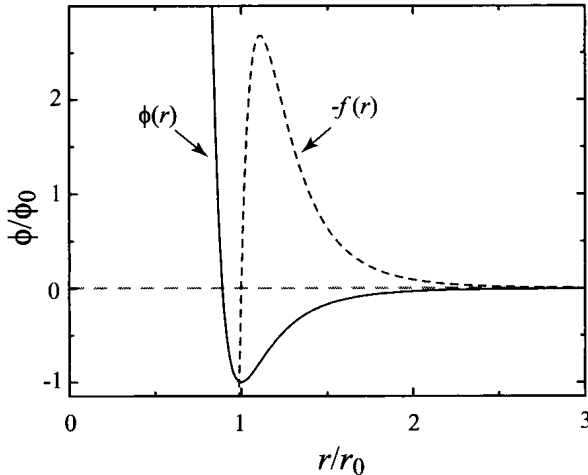


Fig. 1.1. Lennard-Jones model interaction force $-f(r)$ and potential energy $\phi(r)$, as a function of distance r/r_0 . Note we have plotted the negative of the force, so that a positive value corresponds to an attractive force. The vertical axis is for the potential, in units of the potential at the minimum, $\phi_0 = -\phi(r_0)$.

In Fig. 1.1 we have plotted the Lennard-Jones potential $\phi(r)$ and the force $-f(r)$, as a function of distance r , in units of the equilibrium distance $r_0 = (2B/A)^{1/6}$. At $r = r_0$, the force is zero, and equivalently, the potential energy has a minimum. The *binding energy* E_b , the difference between the potential energy minimum and that when the atoms are infinitely far apart, is given by $E_b = \phi(\infty) - \phi(r_0) = A^2/4B$. This amount of energy must be transferred to the atoms in order to break the bond between them.

The Lennard-Jones potential gives an excellent, quantitative description of the interactions between noble gas atoms, such as in argon, krypton and xenon. In argon, for example, the equilibrium spacing in the Ar_2 molecule is found to be $r_0 = 3.8 \text{ \AA}$, and the binding energy is $E_b = 10.4 \text{ meV} = 1.7 \times 10^{-21} \text{ J}$ [1]. Equivalently, we can write down the constants $A = 2r_0^6 E_b = 63 \text{ \AA}^6\text{-eV}$ and $B = r_0^{12} E_b = 9.4 \times 10^4 \text{ \AA}^{12}\text{-eV}$.

The binding energy for argon is less than the thermal energy scale at room temperature, $k_B T = 26 \text{ meV}$. Solid Ar, formed through multiple bonds of the kind we have just described, therefore only forms at quite low temperatures, below 100 K. The van der Waals interaction, with typical binding energies in the 10-100 meV range, is particularly weak; while the equilibrium distance r_0 is typical for all atomic interactions, the binding energy for the much stronger ionic (electrostatic), metallic and covalent interactions in typical solids is in the range of one to several tens of electron volts ($\sim 10^{-19} - 10^{-18} \text{ J}$), rather than a few meV. These types of bonds are however not as simply parameterized as the Lennard-Jones interaction, but require a more sophisticated approach. However, meaningful results can be obtained by simply

increasing the binding energy E_b in the Lennard–Jones potential, in order to mimic these other types of bonds: As we shall see, in most cases it is only the shape of the potential near the minimum in potential energy that determines the important mechanical properties of a solid, and this shape is common to almost all the different bond types.

1.1.1 External Forces

We can now imagine what happens if we try to pull our two atoms apart. Let's say that we apply equal and opposite external forces f_{ext} to each atom. The atoms will move apart until they reach a new equilibrium point r'_0 , where their attractive interaction balances the external force, $-f(r'_0) = f_{\text{ext}}$. If the external force is too large, above the maximum value of $-f(r)$ in Fig. 1.1, there will be no equilibrium point and the atoms will unbind.

Another way to understand this is to define the potential energy associated with the external force, $\phi_{\text{ext}}(r) = -f_{\text{ext}}r$. Note that the zero for the external potential is chosen at $r = 0$. Note there is no factor of two in this expression: Both atoms are acted upon by the external force, but each atom is only displaced from $r = 0$ by $r/2$, so the work done by the force, which is the negative of the potential energy, is $W = 2 \times f_{\text{ext}}r/2$.

The total potential energy is then $U_{\text{tot}} = \phi(r) + \phi_{\text{ext}}(r)$. For $f_{\text{ext}} = 0$, the total potential energy is the same as the interaction potential. For small f_{ext} , the minimum for the total potential U_{tot} will shift to the new equilibrium point r'_0 ; for f_{ext} too large, no minimum occurs. In Fig. 1.2, we show a family of potential energy curves for different external forces, showing how the minimum energy point moves away from r_0 until it disappears at large enough f_{ext} (see Exercise 1.2).

Note that as soon as we apply the external force, the energy minimum at r'_0 becomes *metastable*; the atoms can achieve a lower total energy if they can cross over the potential barrier and escape to infinity. This provides interesting questions in the case where we allow the atoms to have non-zero temperature, so that there is a certain probability that they can be thermally activated over the potential barrier; the same question occurs when we consider quantum mechanical *tunnelling*, through the barrier, also allowing the atoms to escape.

In addition to the question of binding, it is often useful to know how a solid, or in our case, the two atoms, respond to very weak forces, such that the atoms only displace a very small amount from their equilibrium positions, from r_0 to r'_0 . We can use our model Lennard–Jones interaction to see how this works. For a very weak force f_{ext} , the very small shift in the equilibrium point allows us to approximate the interaction potential by using a *Taylor series* expansion of the potential:

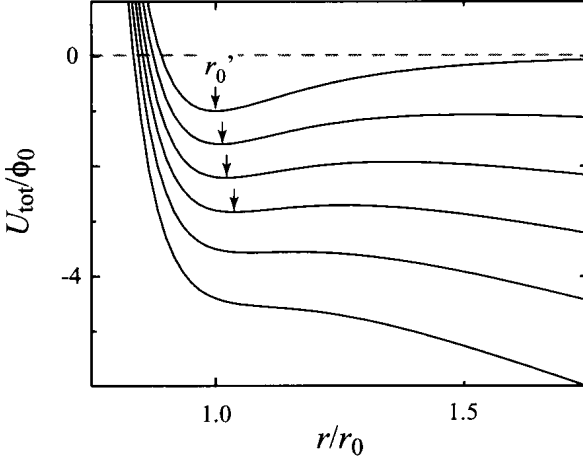


Fig. 1.2. Total potential energy U_{tot} for the Lennard–Jones potential in the presence of a constant external force; the family of curves is for external forces ranging from zero (*top*) to a force larger than the maximum Lennard–Jones binding force (*bottom*). The arrows indicate the new equilibrium point r'_0 for each value of the external force. Vertical axis is in units of the interaction potential at the minimum point.

$$\begin{aligned}
 \phi(r) &= \phi(r_0) + \left. \frac{d\phi}{dr} \right|_{r_0} (r - r_0) + \frac{1}{2!} \left. \frac{d^2\phi}{dr^2} \right|_{r_0} (r - r_0)^2 \\
 &\quad + \frac{1}{3!} \left. \frac{d^3\phi}{dr^3} \right|_{r_0} (r - r_0)^3 + \dots \\
 &\approx \phi(r_0) + \frac{1}{2} \left. \frac{d^2\phi}{dr^2} \right|_{r_0} (r - r_0)^2,
 \end{aligned} \tag{1.5}$$

where in the second, approximate equality, we have used the fact that $d\phi/dr(r_0) = 0$, and we have dropped the higher order terms in the Taylor expansion. We are thus left with a *harmonic potential* approximation for the interaction, that depends quadratically on the square of the displacement $u = r - r_0$ from equilibrium.

For the Lennard–Jones potential, the curvature is given in terms of the equilibrium spacing and binding energy by

$$\left. \frac{d^2\phi}{dr^2} \right|_{r_0} = 72 \frac{E_b}{r_0^2}. \tag{1.6}$$

In Fig. 1.3 we show the harmonic approximation to the Lennard–Jones potential; the approximation is seen to work well for very small displacements from equilibrium, but rapidly fails as one moves further away.

In the presence of a weak external force, the equilibrium point shifts to where $dU_{\text{tot}}/dr = 0$; using the expansion (1.5) for the interaction potential, this is when

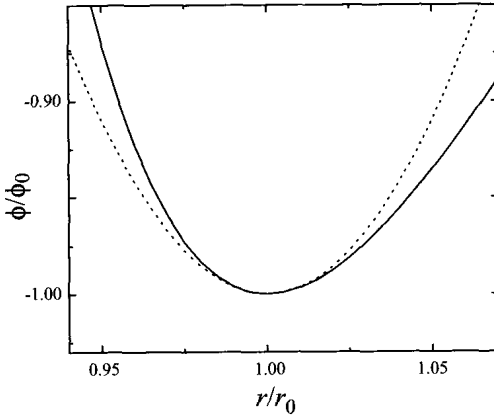


Fig. 1.3. Harmonic approximation (*dotted line*) to the Lennard-Jones potential.

$$-f_{\text{ext}} + \left. \frac{d^2\phi}{dr^2} \right|_{r_0} (r - r_0) = 0, \quad (1.7)$$

or

$$u \equiv r - r_0 = \frac{1}{d^2\phi/dr^2} f_{\text{ext}} = \frac{1}{k} f_{\text{ext}}. \quad (1.8)$$

We thus find that the displacement u from equilibrium, for small forces f_{ext} , is linear in the external force, with a response in inverse proportion to the curvature of the interaction potential $\phi(r)$. The interatomic potential is therefore equivalent to a spring with spring constant k , with restoring force proportional to the displacement. Applied to argon, the curvature, or equivalently the spring constant, is given by $d^2\phi/dr^2(r_0) = 52 \text{ meV/\AA}^2$, with an equivalent spring constant of $k = 0.83 \text{ N/m}$.

The linear response for small displacements u is a generic property of almost all solids, and holds for complex single-crystal materials as well as for amorphous solids made of plastics and proteins.

1.1.2 Dynamic Motion

We now consider the dynamical behavior of the atoms in our model interaction potential. What this means is that we will allow the atoms to move, so that they have a kinetic energy T in addition to the potential energy $U = \phi(r)$.

We assume that the *center of mass* of our system remains at rest. With the atoms at distances r_1 and r_2 from the origin, their separation is $r = r_2 - r_1$. If the atoms have masses M_1 and M_2 , the location of the center of mass r_{cm} is the weighted sum of their locations, or

$$r_{\text{cm}} \equiv \frac{M_1 r_1 + M_2 r_2}{M_1 + M_2}. \quad (1.9)$$