

The Calculation of Phonon Frequencies

G. DOLLING*

CHALK RIVER NUCLEAR LABORATORIES
ATOMIC ENERGY OF CANADA, LIMITED
CHALK RIVER, ONTARIO, CANADA

I. Introduction	1
A. Historical Background	1
B. Basic Equations of Motion	2
C. Interatomic Potentials and Force Models	8
II. Interatomic and Interionic Force Models	10
A. Rare Gas Solids	10
B. Ionic Crystals	12
C. Metals	18
D. Covalent Crystals	21
III. Intermolecular Force Models	23
A. Intermolecular Force Constants	23
B. Expansion in Terms of Interatomic Forces	26
C. Molecular Distortion and Polarization	29
IV. Discussion	30
A. Theoretical and Experimental Approaches to Model Building	30
B. Application of Group Theory	34
C. Limitations and Ambiguities: Utilization of Force Models	35
References	38

The Use of Computers in Scattering Experiments with Slow Neutrons*

R. PYNN

PHYSICS DEPARTMENT, BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK

I. Introduction	41
II. Vocabulary of Neutron Scattering	42
A. The Neutron Scattering Cross Section	42
B. Coherent and Incoherent Scattering	44
C. The Fluctuation Spectrum	45
D. The Time-Dependent Correlation Function	46
E. The Phonon Expansion	47
F. Relation to Subsequent Chapters	48
III. Spectrometers	48
A. Determination of Neutron Energies and Trajectories	48
B. Triple-Axis Spectrometers	50
C. Time-of-Flight Spectrometers	54
D. Correlation Choppers	57
IV. Analysis of Neutron Scattering Data	59
A. Random and Pseudorandom Errors	59
B. Systematic Errors	60
C. Multiple Scattering	61
D. Resolution for a Triple-Axis Spectrometer	62
V. A Note on the Bibliography	72
Appendix: Neutron Scattering Cross Section	72
References	74

Group Theory of Lattice Dynamics by Computer*

JOHN L. WARREN

LOS ALAMOS SCIENTIFIC LABORATORY, UNIVERSITY OF CALIFORNIA
LOS ALAMOS, NEW MEXICO

AND

THOMAS G. WORLTON

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

I. Introduction	78
II. The Equations of Motion and the Space-Time Translation Group	79
A. General Approach and Assumptions	79
B. Atomic Coordinates and the Displacement Fields	80
C. The Lagrangian and the Equations of Motion	83
D. The Space-Time Group	86
E. Generation of the Space Group by Computer Methods	87
F. The Translation Group and the Dynamical Matrix	89
III. The Time Reversal Point Group of the Wave Vector	93
A. Time Reversal and Complex Conjugation	93
B. Transformation of the Eigenvectors and the T Matrices	93
C. The Invariance Group of the Transformed EOM	94
D. Irreducible Multiplier Operator Representations and Decomposition	95
E. Generation of the IMR's by Computer	96
F. Wave Vectors, Brillouin Zones, and Labeling	100
G. Time Reversal Degeneracy	102
IV. Symmetry Reduction of the Dynamical Matrix	105
A. The Self-Consistent Equation for Symmetry Reduction	105
B. Use of Random Numbers	106
C. Conversion of Random Numbers to Symbols for Printout	107
D. Future Developments	108
V. Projection Operators and Symmetry Coordinates	109
A. Definitions	109
B. Examples	110
C. Complications Caused by Time Reversal Invariance	112
VI. Block Diagonalization of the Dynamical Matrix	113
A. Advantages	113
B. Procedure	114
VII. Optical Selection Rules and Acoustic Mode Identification	115
A. Optical Selection Rules	115

* Work supported by the U.S. Atomic Energy Commission.

B. Acoustic Mode Identification 116
C. A Problem of Optic Modes at the BZ Center 116
VIII. Some Uses of Symmetry Coordinates 117
References 117

Lattice Dynamics and Related Properties of Point Defects*

R. F. WOOD

SOLID STATE DIVISION, OAK RIDGE NATIONAL LABORATORY
OAK RIDGE, TENNESSEE

I. Introduction	119
A. Introductory Comments	119
B. Localized Perturbation Theory and the Coherent Potential Approximation	121
C. Scope of the Article	122
II. Measurable Quantities in Terms of Single-Particle Green's Functions	123
A. Far Infrared Absorption	123
B. Anharmonic Sidebands of Local Modes	124
C. Raman Scattering	125
D. Neutron Scattering	128
III. Localized Perturbations	129
A. Outline of Localized Perturbation Theory	129
B. Defect Space and Symmetry Coordinates	131
C. Green's Functions, Projection Operators, and Overlap Integrals	134
D. Transformation Properties of Overlap Integrals and Green's Functions	138
E. The Coherent Potential Approximation	140
IV. Computational Considerations	143
A. Outline of a Typical Calculation	143
B. Extent of the Defect Space	145
C. Brillouin Zone Integration	146
D. Comments on Computer Time and Storage	148
V. Comparison between Theory and Experiment	149
A. Infrared Studies of the H^- Ion in Alkali Halides	149
B. Infrared and Raman Studies of $NaCl:Ag^+$	153
C. Neutron Scattering from Dilute Alloys	156
References	160

Lattice Dynamics of Surfaces of Solids*

F. W. DE WETTE AND G. P. ALLDREDGE[†]

DEPARTMENT OF PHYSICS
THE UNIVERSITY OF TEXAS
AUSTIN, TEXAS

I. Introduction	163
A. General Remarks	163
B. Overview of the Computational Methods	166
C. Crystal Models Used	168
II. Formulations	169
A. Lattice Dynamics of a Crystal Slab and Its Direct Solution	170
B. Molecular Dynamics of a Crystal Slab	181
C. Matching Method	182
D. Green Function Method	185
III. Results	187
A. Surface Structure (Relaxation)	188
B. Surface Phonon Spectra	188
C. Derived Physical Quantities	197
References	210

Vibrational Properties of Amorphous Solids

R. J. BELL

DIVISION OF QUANTUM METROLOGY
NATIONAL PHYSICAL LABORATORY
TEDDINGTON, MIDDLESEX, ENGLAND

I. Introduction	216
II. Equations of Vibrational Motion	218
A. Quantum-Mechanical Equations of Motion	218
B. Classical Equations of Motion	221
C. Matrix Notation for Equations of Motion	222
D. The Green's Function	224
E. Density of States	225
III. Properties of Regular Lattices and Lattices with Point Defects	226
A. Matrix Reduction Theorem for Perfect Lattices	226
B. Linear Chains and Simple Lattices	228
C. Lattice Green's Functions	230
D. The Perturbed Green's Function	230
E. Localized Defects	232
F. Isolated Mass Defects in Simple Lattices	232
IV. The Numerical Determination of Frequency Spectra	235
A. The Negative Eigenvalue Theorem	236
B. Calculation of Selected Eigenvalues	238
C. Eigenvectors	239
D. Computational Aspects	241
V. Vibrational Spectra of Noncrystalline Solids	243
A. Two-Component Mass Disordered Chains and Lattices	244
B. One- and Two-Dimensional Glasses	248
C. Real Three-Dimensional Glasses	250
VI. Interaction with Radiation	253
A. Neutron Scattering	254
B. Infrared Absorption	257
C. Raman Scattering	260
VII. Description of the Normal Modes	266
A. Fourier Analysis	266
B. Normal Mode Assignments	267
C. The Spatial Extent of Modes	270
D. Optical and Acoustic Characteristics of Modes	272
VIII. Concluding Remarks	274
References	274

Lattice Dynamics of Quantum Crystals

T. R. KOEHLER

IBM RESEARCH LABORATORY
SAN JOSE, CALIFORNIA

I. Introduction: Unique Aspects of Quantum Solids	277
II. Necessary Theoretical Tools	280
A. Formulation of the Problem	280
B. Self-Consistent Phonon Theory	282
C. Anharmonicity	286
D. Hard-Core Problems	289
III. Theories	290
A. Jastrow Function Variational	290
B. Correlated Basis Function	291
C. t -Matrix Theories	293
D. Fully Consistent Theories	295
IV. Comparison with Experiment	299
A. Ground-State Energy Results	299
B. Phonon Properties	302
C. Interference Effects	309
V. Conclusions and Future Prospects	312
References	313

Methods of Brillouin Zone Integration

G. GILAT

DEPARTMENT OF PHYSICS
TECHNION—ISRAEL INSTITUTE OF TECHNOLOGY,
HAIFA, ISRAEL

I. Introduction	317
A. The Basic Problem	317
B. Relationship between Computation and Observation	320
II. Methods of Zone Integration	325
A. Root Sampling	326
B. Discrete Methods	328
C. Analytical (Continuous) Method	331
D. Combined (Hybrid) Method	337
E. Interpolation and Extrapolation Methods	341
F. Analysis of Resolution, Accuracy, and Computing Effort	344
G. Transition Probabilities	347
H. Real Part Calculations	350
III. Examples of Spectral Properties in Solids	352
A. Phonon Densities of States	352
B. Tunneling	355
C. Phonon Sidebands	356
D. Second-Order Raman Effect	358
IV. Other Problems Related to Zone Integration	360
A. Lifetime Effects	360
B. Two Excitation Transitions (e.g., Photoemission)	363
C. Derivatives of Spectral Functions	364
D. Meshes and Shapes of Integration Cells	365
V. Summary and Conclusions	367
References	368

Computer Studies of Transport Properties in Simple Models of Solids*

WILLIAM M. VISSCHER

THEORETICAL DIVISION
LOS ALAMOS SCIENTIFIC LABORATORY, UNIVERSITY OF CALIFORNIA
LOS ALAMOS, NEW MEXICO

I. History and Introduction	371
A. The Boltzmann Equation	371
B. Green-Kubo Formulas	373
C. Computer Models	373
II. Thermal Conductivity	374
A. Harmonic One-Dimensional Chains	375
B. Anharmonic Ordered One-Dimensional Chains	379
C. Effects of Computational Errors	394
D. Other Numerical Experiments	396
E. Discussion	398
III. Electric Conductivity	398
A. Model Criteria	399
B. Linear Response Theory	399
C. Conductivity Calculation	400
D. Discussion	403
Appendix: Time-Correlation Function Adapted to Computer Experiments	405
References	407