MASTER

C00-3161-59

MASTER

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

FINAL SUMMARY REPORT

James A. Krumhansl

Laboratory of Atomic and Solid State Physics

Cornell University

Ithaca, New York 14853

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *EB*

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

This is a summary final report of the work done in a series of years from 1960 until 1978 under support by AEC, ERDA and DOE grants in the general subject area of theoretical solid state physics. The subject matter of the field, of course, has evolved over this long period and as the field evolved so has the content of the research program. The best documentation of what has been done is contained in the list of publications and activities which follow as an appendix to this overview discussion.

During the earliest part of the contract period, that is, during the early 1960's the main interest was in two topics. First, the subject of thermal transport by solids was an extremely active one at Cornell and other places, particularly with regard to the effects of impurities on the low temperature thermal conductivity of solids and on the role of anharmonicity in thermal transport. The foundations for the latter had been laid conceptually by Peierls during the 1930's; however, it was to be only 20 years later when the experimental techniques and the theoretical methodology began to allow a quantitative comparison between theory and experiment. The publications during the period 1960 and 1963 were concerned with such matters as the scattering of phonons by lattice defects. During this period several significant applications of modern scattering theory, particularly to determine both resonances and free vibrations of impurities in crystal lattices, were exploited both theoretically and experimentally. In particular the experimental program of Pohl and Sievers were coordinated with the theoretical studies of Krumhansl, Matthew, Takeno and several graduate students. Such studies gave information which was of use not only from the point of view of being basic research on solid state phenomena but also in general as a technique of use in materials science and metallurgy where the role of defects is extremely important.

During the same period and in parallel with the studies of the effect of the defects on lattice vibrations we examined the foundations of thermal transport using methods which had been developed in many body theory. In particular the work of Carruthers adapted to the subject of thermal conductivity the diagrammatic techniques

of quantum field theory, and subsequently the work of Horie and Krumhansl established in a formal manner the Boltzmann equation on a deductive basis rather than the phenomenological basis which had been used until that time. These examinations of the foundations of phonon transport as described by the phonon Boltzmann equation also led to a recognition that phonon transport in perfect crystalline solids (as Peierls had pointed out many years earlier) would allow the possibility of infinite thermal conductivity in the absence of defects. Put another way, the infinite thermal conductivity was the manifestation of wavelike propagation of heat rather than diffusive propagation of heat, and in fact that wavelike propagation was quite analogous to the phenomena of second sound in liquid helium. Prohovsky, Guyer, and Krumhansl particularly developed a formal structure which not only described second solid excitation but, of particular importance, defined the conditions on relaxation times (normal and umklapp) under which the phenomenon might be observed. This statement was in the form of a frequency window, and has been the standard viewpoint for the design of experiments on second sound since that time. The first experimental observation of second sound in a solid was indeed guided by a student Robert Guyer, who, upon leaving Cornell, became a staff member at Duke University where the experiments were carried out on solid helium. Subsequently, Pohl and his students observed second sound in sodium fluoride.

Several other offshoots of this study of the fundamentals of phonon excitations and transport in solids were also studied during that time. Carruthers, although his main interest was in particle physics, continued to work on the topic and developed some fundamental ideas on coherent states and their role for the description of various phenomena in phonon transport. Two students in particular pursued that line, K.S. Dy and Michael M. Nieto.

It can be said that by 1967 the subject of ordinary thermal transport, anharmonic effects, second sound, and the properties of single defect lattice phonon scattering or vibrations all were quite well understood. It was natural at this point then to look at more difficult problems and some of these are to be found in two directions.

One obvious generalization was that of highly disordered solids. The other generalization was to solids which were so anharmonic that they might in fact ordinarily be thought to be unstable, for example the so called quantum crystals solid helium and solid hydrogen. So the direction of the research during the period following 1967 followed those lines.

The program at Cornell contributed significantly to the development of descriptions of disordered alloys, of polycrystalline materials, and such. This covered work on electronic properties, optical properties and lattice vibration properties. The subject was very active during the period of 1968 to 1972 and a thorough exploration of such methods as the coherent potential approximation was carried out at Cornell as well as at many other institutions. Our particular contribution was to systemize and compare the parallel work being done in several branches of the field of solid state physics at that time and to extend the coherent potential approximation from that of a single site description to multiple site phenomena. In this way, to a certain degree, the structure around the defect as well as the defect itself could then be incorporated in an average description of a material containing significant, that is finite, concentration of such defects. This phase of the work was summarized in an extensive review in the Reviews of Modern Physics, coauthored with Elliot of Oxford and Leath of Rutgers.

The other direction taken during the late 60's and early 70's concerned the properties of quantum crystals as noted above. Fundamental calculations were made on the thermal conductivity of neon, helium and argon crystals and a program to investigate the stability of rare gas solids and of hydrogen and helium was begun. Actually significant effort directed toward the properties of solid helium was carried out elsewhere and we chose to concentrate on solid hydrogen because of the then developing interest in the possibility of metallic hydrogen at very high pressure. In this regard, it is important to note that in order to calculate the phase transition from molecular to metallic solid hydrogen it is important not only to know the

properties of the metallic form but also the constitutive relation (i.e. pressure, volume, free energy) of the molecular form. We showed that the methods of quantum crystals could be applied to this problem and work at Cornell was carried out by the principal investigator with a student, Wu, and collaboratively with G.V. Chester and his student, Bruce. Subsequently, two postdoctoral research associates, Beck and McMahan, together with Krumhansl investigated a particularly important fundamental question, namely, what is the form of the potential interaction between molecules of hydrogen at distances small compared to those found at ordinary pressures. This was important because it was not clear that the simple Lennard-Jones form of the interaction would be adequate to describe the intermolecular interaction at the short distances to be expected prior to the metallic transition. This work was subsequently published in the Journal of Chemical Physics and represents one of the best descriptions of the interactions of hydrogen molecules at high densities. During the course of these studies we recognized that although it was necessary at low densities to use the quantum crystal description of materials such as the solid rare gases this was not necessary at high densities and indeed that it would be possible to approximate the equations of state quite well by the standard classical methods; E.L. Pollock, T.A. Bruce, G.V. Chester and J.A. Krumhansl collaborated on numerical and theoretical studies of this question.

As frequently happens there are offshoots of a piece of research directed toward one goal. In this instance the studies of interactions of molecules or rare gas atoms in the solid form stimulated our interest in liquids, and two students, S.S. Wang and W. Kerr, addressed certain aspects of the theory of liquids. While this did not constitute a long term activity in the program, it was possible to obtain a deeper understanding of the superposition assumption (Kirkwood) which had been commonly used in the theory of liquids, and to develop a heuristic description of the excitation spectrum of liquid helium in a framework which combined quasi particle

and phonon like excitations. Again, the topics of interest in solid state physics and materials science evolved and new phases of the work were begun in 1973.

We began a systematic exploration of some of the macroscopic engineering properties of polycrystalline materials borrowing the methodology which had been developed in materials which are disordered at the atomic scale. It was possible to predict accurately the elastic constants of polycrystalline alloys, rocks, etc., and these methods have been taken over somewhat in theoretical mechanics and other engineering situations.

Then, in 1973, began one of the most important phases of the research. As noted above, the theme of anharmonicity, in particular anharmonicity so extreme that the basic solid structure might be unstable were it not for thermal effects, has been a recurring concern. During a sabbatic leave, in joint work with J.R. Schrieffer at the University of Pennsylvania, we finally addressed the problem of introducing nonlinear effects at the outset with as few approximations as possible, rather than using perturbation theory from a basically harmonic description, which had characterized the subject for fifty years. In particular, we found the extensive literature on solitons and other highly stable nonlinear excitations, which are localized in space and are stable against extended phonon excitations, to be of direct relevance to the exact description of highly anharmonic systems. Since that time there has been an extensive series of investigations and publications covering the statistical mechanics, the possible structural transitions, questions such as the dynamics near phase transitions and the central peak, the possibility of solitonic excitations in the condensed Peierls state in one-dimensional materials, and the role of solitary excitations as mechanisms in epitaxy, in the omega phase transition in zirconium niobium alloys, and in discommensuration of charge-density waves. This past five year period has been a rich one from the point of view of research subject, it is quite certain that in inelastic neutron scattering studies, and in structural studies by electron diffraction and

by x-ray diffraction the proper description of many phenomena lies in the combination of solitary nonlinear excitations with the more traditional phonon like excitations of solids.

This summary should provide an overview and perspective for the list of publications which follows. It is fair to say that the topics which have evolved over the course of this contract have kept pace with the forefront of the field of material science and represent a significant increase in our understanding of basic properties, as well as providing a base for many applications in materials science.

It is important to close with an acknowledgment of the continued generous support and confidence which we have had from our sponsors over this period.

PUBLICATIONS

- P. Carruthers, Resonance in Phonon Phonon Scattering, Phys. Rev. 125, 123, 1962.
- P. Carruthers, Thermal Conductivity of Solids III, Modification of the Three Phonon Processed by Isotopic Scattering, Phys. Rev. 126, 1448, 1962.
- P. Carruthers and How-Sen Wong, Photoproduction of Pion Pairs near Threshold, Phys. Rev. 128, 2382, 1962.
- P. Carruthers and A. Griffin, Resonance Fluorescence Scattering of Phonons by Donor Electrons in Semiconductors, published in Phys. Rev. 1962.
- C. Horie and J. A. Krumhansl, "Boltzmann Equation in a Phonon System," Phys. 136, A1397 (1964).
- J.A. Krumhansl, "Thermal Conductivity of Insulating Crystals in the Presence of Normal Processed," submitted to Proc. Phys. Soc. (London).
- C. Julian, "Theory of Heat Conduction in Rare Gas Crystals." THESIS
- R.A. Guyer, "Boltzmann Equation Treatment of Time Dependent Thermal Conduction in Non-Metallic Crystals." THESIS
- J.A. Krumhansl and J.A.D. Matthew, "Scattering of Long Wavelength Phonons by Point Imperfections in Crystals" Phys. Rev. 140, A1812, (1965).
- R.A. Guyer and J.A. Krumhansl: "Thermal Conductivity, Second Sound, and Phonon Hydrodynamic Phenomena in Non-Metallic Crystals", Phys. Rev. 148, 778, 1966.
- J.A.D. Matthew, "Properties of Small Ions in Ionic Host Lattices", Solid State Communications 3, 365(1965).
- A. Griffin, "The Effect of Large Uniaxial Stress on Resonant Phonon Scattering in N-type Germanium", J. Phys. Chem. Solids 26, 1909(1965).
- J.A.D. Matthew, "An Approximate Technique for Calculating Localized Modes", J. Phys. Chem. Solids 26, 2607(1965).
- P. Carruthers and M.M. Nieto, "Coherent States and the Number-Phase Uncertainty Relation", Phys. Rev. Letters 14, 387(1965).

- P. Carruthers and M.M. Nieto, "Coherent States and the Forced Quantum Oscillator", Am. J. Phys. 33, 537(1965).
- A.J. Sievers and S. Takeno, "Isotope Shift of a Low-Lying Lattice Resonant Mode", Phys. Rev. 140, A1030(1965).
- S. Takeno and A.J. Sievers, "A Characteristic Temperature Dependence for Low Lying Lattice Resonant Modes", Phys. Rev. Letters 15, 1020(1965).
- S. Takeno, "Exciton Impurity States in Molecular Crystals" J. Chem. Phys. (to be published in Feb. 1966).
-
- "Coherent States and Irreversible Processes in Anharmonic Crystals", P. Carruthers and K.S. Dy, Phys. Rev. 147, 1, 214 (1966).
- "Solution of the Linearized Phonon Boltzmann Equation", R.A. Guyer and J.A. Krumhansl, Phys. Rev. 148, 2, 766 (1966).
- "Thermal Conductivity, Second Sound and Phonon Hydrodynamic Phenomena in Nonmetallic Crystals", R.A. Guyer and J.A. Krumhansl, Phys. Rev. 148, 2, 278 (1966).
- "Physical Properties of an Off-center Impurity in the Tunneling Approximation I. Statics", M. Gomez, S.P. Bowen, J.A. Krumhansl, Phys. Rev. 148, 2, 778 (1966).
- "Theory of Displaceable Point Defects in Crystals", S.P. Bowen, M. Gomez, J.A. Krumhansl and J.A.D. Matthew, Phys. Rev. Letters 16, 24, (1966).
- "Vacancy Formation Energy and Debye Temperature in Close Packed Metals", N.H. March, Phys. Letters, 20, 3, (1966).
-
- "Dynamical Model for Negative Parity Regge Trajectories in the Pion Nucleon System", P. Carruthers and Martin M. Nieto, Phys. Rev. Letters, 18, 297 (1967).
- "High Spin Baryons. II. Dynamical Mechanisms for Regge Recurrences of Inelastic Resonances: General Theory", P. Carruthers, Phys. Rev. 154, 1399 (1967).
- "Locality and the Isospin of Self-Conjugate Bosons", P. Carruthers, Phys. Rev. Letters 18, 353 (1967).
- "An Asymptotic Description of Localized Lattice Modes and Low-Frequency Resonances", J.A. Krumhansl and J.A.D. Matthew, Phys. Rev. Feb. 15, 1968.
- "Asymptotic Descriptions of Defect Excitations", J.A. Krumhansl, Irvine Conference on Localized Excitations, September 1968.

- "Phase and Angled Variables in Quantum Mechanics", P. Carruthers and Michael M. Nieto, *Rev. Mod. Phys.* 40, 441 (1968).
- "Coherent State and its Applications to Quantum Statistical Mechanics", Kian Seng Dy, Ph.D. Thesis.
- "Effects of Impurities on Lattice Vibrations on Model Calculations Including Mass and Force Constant Changes Neutron Scattering", Katja Lakatos, Ph.D. Thesis.
- "Infrared Absorptions of Substitutional Impurities in Alkali Halides", Richard Chu-Tak Tseng, Ph.D. Thesis.
- "The Dynamics of a Non-harmonic Substitutional Impurity in a Dynamic Host Lattice", S.P. Bowen, Ph.D. Thesis.
- "A Model Calculation of the Liquid Structure Factor in Liquid Helium-4", William C. Kerr, Ph.D. Thesis.
- "A Calculation of Phonon Lifetimes in Solid Argon", Hilary D. Jones, Ph.D. Thesis.
- "Physical Properties of off Center Impurities", M. Gomez, Ph.D. Thesis.
-
- "On the Hard-Core Renormalization in the Lattice Dynamics of Quantum Crystals," G. Meissner, *Phys. Letters* 27A, 261 (1968), (NYO-3699-25).
- "Dispersive Anharmonic Effects in the Lattice Dynamics of Quantum Crystals with Hard Core Potentials," G. Meissner, *Phys. Rev. Letters* 21, 435 (1968), (NYO-3699-28).
- "Dispersive Anharmonic Effects in Lattice Dynamics of Solid Helium," Proceedings of the Eleventh International Conference on Low Temperature Physics, St. Andrews, 1968 (NYO-3699-30).
-
- "Effect of Force-Constant Changes in Incoherent Neutron Scattering from Cubic Crystals with Point Defects," K. Lakatos and J. A. Krumhansl, *Phys. Rev.* 175, 841 (1968)
-
- "A Dynamic Exchange Coupling in Ferroelectric KDP," J. A. Krumhansl, submitted to *Phys. Rev. Letters*, returned for revision, in progress (NYO-3699-26).
- "Dynamics of Soft Mode Systems Near T_c ," R. J. Elliott and J. A. Krumhansl, for "Comments on Solid State Physics," probably mid 1969 (in draft).
- "Thermal Conductivity of Ne and He^4 Quantum Crystals," D. B. Benin, *Phys. Rev. Letters* 20, 1352 (1968); work begun at Univ. of Rochester, completed at Cornell. Publication supported under U. S. Air Force OSR.

"Atomic Tunneling in Solids," J. A. Krumhansl, (1969, p. 551
Plenum Press (NYO-3699-22).

"Electric Field Induced Dichroism of CN^- Molecules in Alkali Halides," R. Pompei and V. Narayanamurti, Solid State Communications 6, 645 (1968), (NYO-3699-27).

"On the Theory of Quantized Vortices," G. V. Chester, R. Metz, and Reatto, L., Phys. Rev. 175, 275 (1968). (NY)-3699-9).

"Self-Consistent Approximations for the Heisenberg Model," R. B. Stinchcombe, submitted to the Proceedings of the Physical Society of London (NYO-3699-31).

"Collective Modes of Vortex Lattices," L. Reatto, Phys. Rev. 167, 191 (1968), (NYO-3699-9).

Miscellaneous

The principal personnel on the program are mentioned above.

In addition we had R. J. Elliott, Oxford, visiting and working on the program during August 1968. Graduate student activity was minimal, due to previous sabbatic leaves of principal investigators; new students have joined the program now. Thus, though the contract will be underspent this contract year, it will be up to full level in 1969-70.

(NYO-3699-33) "Effect of Force-Constant Changes on the Coherent Neutron Scattering from Face-Centered Cubic Crystals with Point Defects," K. Lakatos and J. A. Krumhansl, Phys. Rev. 180, 729 (1969).

(NYO-3699-34) "Pair Effects and Self-Consistent Corrections in Disordered Alloys," R. J. Elliott, R. N. Aiyer, P. L. Leath, and J. A. Krumhansl, Phys. Rev. 181, 1006 (1969).

(NYO-3699-36 and NYO-2391-91) "Theory of the Electric Field from Phonons Perturbed by Substitutional Impurities in Ionic Crystals," Phys. Rev. 184, 905 (1969), J. B. Page, Jr.

(NYO-3699-37) "The Phase Transition in the Pair Hamiltonian Model for Liquid Helium," L. Reatto and J. P. Straley, Phys. Rev. 183, 321 (1969).

(NYO-3699-38) "Effective Ion-Ion Interaction in Liquid Metals," Physics of Simple Liquids, North Holland Publ. Co., Amsterdam, 1968, N. H. March.

(NYO-3699-39) "Crystallization and Instabilities in Highly Anharmonic Crystals," to be published in Phys. Rev., Gunther Meissner.

(NYO-3699-40) "Monte Carlo Calculations of the Density Dependence of Sound Velocities in Solid Neon," Phys. Letts. 30A, 61 (1969), G. Meissner and Jean-Pierre Hansen.

(NYO-3699-41) "Raman Scattering as a Probe of Pure Crystal Phonons in Tl^+ Doped Potassium Halides," Phys. Rev. Letters 23, 922 (1969), John B. Page, Richard T. Harley and Charles T. Walker.

(NYO-3699-42) "Ground State of the Inhomogeneous Bose Liquid," David Hyman (Ph. D. Thesis).

(NYO-3699-43) "An Equation of State for Solid Hydrogen," T. Bruce, (Masters Thesis); joint with G. V. Chester under NSF and ARPA support.

(NYO-3699-44) "Debye Temperature and Second Sound Velocity of Solid He^{44} ," Stanley A. Strauss, for submission to Solid State Communications.

(NYO-3699-45) "Improved Variational Principles for Transport Coefficients," to be published in Phys. Rev., March 15, 1970, D. Benin.

(NYO-3699-48) "Raman Scattering in Resonance with the Exciton Transition in Pure Polar Crystals", E. Muzazzi (with M. Fontana), Phys. Rev. Letters 25, 228 (1970).

(NYO-3699-51) "The High Pressure Behavior of Solid H_2 , D_2 , He^3 , He^4 , and Ne^{20} ," E. L. Pollock, T. A. Bruce, G. V. Chester, and J. A. Krumhansl, Phys. Rev. B5, 4180 (1972).

(NYO-3699-52) "An Equation of State for Solid Hydrogen," Thomas Alexander Bruce, Phys. Rev. B5, 4170 (1972).

"Ground-State Properties of Solid Helium-4 and -3," J.P. Hansen and E. L. Pollock, Phys. Rev. A5, 2651 (1972).

"Liquid-Helium Configuration around a Metastable Excited Helium Atom," J.P. Hansen and E.L. Pollock, Phys. Rev. A5, 2214 (1972).

(NYO-3699-50) "Influence of Two-Body Potential on Ground-State Properties of Solid Helium," by J. P. Hansen, Physics Letters 34, 61 (1971).

(NYO-3699-49) "Effect of Disorder on the Band Structure of SiGe," D. Stroud and H. Ehrenreich, in Proceedings of the International Semiconductor Conference at Cambridge, 1970.

(NYO-3699-47) "Phase Stability in Binary Alloys," D. Stroud and N. W. Ashcroft, J. Phys. F (Proc. Phys. Soc.) (In press).

"Pair Effects and Random Lattices: A Generalized C.P.A. and its Equivalence to Diagrammatic Expansions", B.G. Nickel and J.A. Krumhansl, Phys. Letters, 36A, 111 (1971).

"Self-Consistent Average Green's Function in Random Lattices: A Generalized Coherent Potential Approximation (n) and its Diagrammatic Equivalents", B.G. Nickel and J.A. Krumhansl, Phys. Rev. B4, 4354 (1971).

"A Note on the Two-Dipole Problem", M.J. Mandell, Solid State Comm. 9, 1323 (1971).

"The Superposition Assumption I: Low Density Fluid Argon", J.A. Krumhansl and Shein-shion Wang, J. Chem. Phys., March 1972.

The Superposition Assumption II: High Density Fluid Argon", Shein-shion Wang and J.A. Krumhansl, J. Chem. Phys.

"Liquid Helium Correlation Around a Metastable Excited Helium Atom", J.P. Hansen and E.L. Pollock, Phys. Rev., May 1972.

"Ground State Properties and Low Excited States of Solid Helium-4 and -3", J.P. Hansen and E.L. Pollock, Phys. Rev., May 1972.

"Note on the Band Gaps of Semiconductor Alloys", David Stroud, AT(30-1)-3699, AEC Report NYO-3699-61 (1971).

"Theory of the Melting of Simple Metals: Applications to Na", D. Stroud and N.W. Ashcroft, Phys. Rev. B5, 371 (1971).

"Validity of the Boltzmann Equation for Systems with both Electron-Phonon and Impurity Scattering", B.G. Nickel and .W. Wilkins, AEC Report NYO-3699-56, (1971).

"Evaporation of Cold Metallic Hydrogen", E.E. Salpeter, Phys. Rev. Letters 28, (1972).

"Quantum Theory of the Equation of State for Solid Hydrogen", J.A. Krumhansl and S.Y. Wu, Phys. Rev., April 1972.

"Dynamic Susceptibility of a Model Polymer in Several Limits -- Theory and Calculations", M. J. Mandell, J. Chem. Phys. 57, 4858, 1972.

"Approximate Phonon Frequency Distributions for FCC Lennard-Jones Harmonic Crystals", E. L. Pollock,

"Pair Potential in Liquids From The Exact Born-Green Equation: I. Model Testing", S. Wang and J.A. Krumhansl, J. Chem. Phys. 57, 4202, 1972.

"Theory of Phase Separation in Liquid Metal Alloys: $\text{Li}_{\text{x}}\text{Na}_{1-\text{x}}$ ", D. Stroud

"Feynmann Graph Expansions for Critical Exponent

"Static and Dynamic Properties of Systems with Multipole Interactions and Internal Dynamic Structure", M.J. Mandell, THESIS

- "Critical Exponents For Long-Range Interactions", Michael E. Fisher, Shang-keng Ma and B.G. Nickel, Phys. Rev. Lett. 29, 917 1972.
- "Problems in Strong Scattering Binary Alloys", Bernie G. Nickel, William H. Bulter, Phys. Rev. Lett. 30, 373, 1973.
- "Dynamic Effects in the Collective Excitations of Singlet-Triplet Particles", M. J. Mandell
- "It's a Random World", J.A. Krumhansl, Reprinted from AMORPHOUS MAGNETISM, Plenum Publishing, 1972-73.
- "Computer Study of A Classical Quadrupole Solid", M.J. Mandell, J. Chem. Phys. 60, 1432, 1974.
- "Heat Pulse Propagation in Dielectric Solids", H. Beck and R. Beck, Phys. Rev. B8, 1669 1973.
- "Orientational Properties of the Classical One-Dimensional Multipolar Array", M. Mandell, J. Chem. Phys. 59, 3255, 1973.
- "One-Phonon Spectral Function for Solid Helium", A.K. McMahan and H. Beck, Phys. Rev. A8, 3247, 1973.
- "The Theory and Properties of Randomly Disordered Crystals and Related Physical Systems", R.J. Elliott, J.A. Krumhansl and P.L. Leath, Reviews of Modern Physics, Vol. 46, No. 3, July 1974.
- "Spin-Wave Spectrum of Heisenberg Ferromagnets with Random Exchange", J.E. Gubernatis, Phys. Rev. B10, 4025, 1974.
- "Weak Coupling Theory of Paraelectric Absorption Spectra", R. Pirc and B.G. Dick,
- "The Onset of Superfluid in Thin Helium Films", J.M. Kosterlitz,
- "Critical Scattering Parameters for General Fields and Temperatures", M. Combescot, M. Droz and J.M. Kosterlitz, Phys. Rev. Letts., Vol. 33, No. 12, p. 705, 1974.
- "Macroscopic Engineering Properties of Poly-Crystalline Materials. Elastic Properties", J.E. Gubernatis and J.A. Krumhansl, Jour. of Appl. Physics, Vol. 46, No. 5, 1975.
- "Two Point Correlation Function for General Fields and Temperatures in the Critical Region", M. Combescot, M. Droz, J.M. Kosterlitz, Phys. Rev. B11, 4661, 1975.
- "Notes on the Main Band Fine Structure of a Dilute, Disordered Binary Chain", J.E. Gubernatis and S.Y. Wu, Solid State Comm. 15, 1915, 1974.
- "On the Equivalence of Configurational Averaging Formalisms in the CPA: Two-Particle Properties", A.R. Bishop, Solid State Phys. 8, 1975.
- "Stochastic Theory of Spin-Phonon Relaxation", R. Pirc and J.A. Krumhansl, Phys. Rev. B11, 4470, 1975.
- "On The Equivalence of Configurational Averaging Formalisms in the CPA: Two-Particle Properties", A. R. Bishop, J. Phys. C: Solid State Phys. 8, 1975.

"Dynamics and Statistical Mechanics of a One-Dimensional Model Hamiltonian for Structural Phase Transitions", J.A. Krumhansl and J. R. Schrieffer, Phys. Rev. B11, 3535 (1975).

"Potential Energy and Force Constants of a Potassium Chloride Molecule from Extended Hückel Calculations", Kristl B. Hathaway and J. A. Krumhansl, Journal of Chemical Physics, 63, 10, 1975.

"The Elasticity of Polycrystals and Rocks", E. Domany, J. E. Gubernatis, J. A. Krumhansl, Journal of Geophysical Research, 80, 35, 1975.

"Mean Field and Exact Results for Structural Phase Transitions in 1-D and Very Anisotropic 2-D, 3-D Systems", A. R. Bishop and J. A. Krumhansl, Phys. Rev. B12, 2824 1975.

"Extended Hückel Calculation of Repulsive Interactions in Noble Gases", Kristl B. Hathaway and J. A. Krumhansl, Journal of Chemical Physics, 63, 10, 1975.

"Comments on Dilute Ising Systems", A. R. Bishop and E. Domany, (preprint)

"Absence of Localization in the Coherent Potential Approximation: The One-Dimensional Limit", A. R. Bishop, Solid State Comm. 17, 1405, 1975.

"Remarks on the Structure and Properties of TTF-TCNQ", J. A. Krumhansl and A. R. Bishop (preprint)

"Nonlinear Excitations in Anisotropic X-Y Models", A. R. Bishop and J. F. Currie, Physics Letters 56A, 333, 1976.

"Molecular Dynamics Simulation of a Model For (One-Dimensional) Structural Phase Transitions", T. R. Koshler, A. R. Bishop, J. A. Krumhansl, J. R. Schrieffer, Solid State Comm. 17, 1515, 1975.

"Classical and Statistical Mechanics of Nonlinear Fields with Application in Condensed Matter Physics", John Currie. THESIS

"Weakly Pinned Fröhlich Charge-Density-Wave Condensates: A New, Nonlinear, Current-Carrying Elementary Excitation", M. J. Rice, A. R. Bishop, J. A. Krumhansl, S. E. Trullinger, Phys. Rev. Letters, 36, 2 1976.

"The Fundamental Theory of Elastic Wave Scattering by Defects in Elastic Materials-Integral Equation Methods for Application to Ultrasonic Flaw Detection", J. E. Gubernatis, E. Domany, J. A. Krumhansl, M. Huberman, Materials Science Center, Report Number 2654, 1976.

"Quantum Corrections to Domain Walls in a Model (One-Dimensional) Ferroelectric", A. R. Bishop, E. Domany, J. A. Krumhansl, Physical Rev. B., 14, 7, 2966, 1976.

"Adaptation of Semiempirical Molecular Orbital Methods for Dynamic Calculations in Ionic Molecules and Non-Metallic Solids", Kristl B. Hathaway. THESIS

"Classical Particle-Like Behavior of Sine-Gordon Solitons in Scattering Potentials and Applied Fields", A. R. Bishop, M. B. Fogel, S. E. Trullinger, J. A. Krumhansl, Physical Rev. Lett., 36, 24, 1411, 1976.

"Dynamics of Sine-Gordon Solitons in the Presence of Perturbations", A. R. Bishop, M. B. Fogel, S. E. Trullinger, J. A. Krumhansl, Phys. Rev. B15, 1578, 1977.

"A Combined Bond-Site Percolation Problem", Paul Muzikar (preprint)

"Microscopic Derivation of Domain Walls", E. Domany, A. R. Bishop, J. A. Krumhansl, Ferroelectrics, 16, 183, 1977.

"The Born Approximation in the Theory of the Scattering of Elastic Waves by Flaws", E. Domany, J. E. Gubernatis, J. A. Krumhansl, M. Huberman, J. of Applied Physics, 48, 2812, 1977.

"Solitary-Wave Solution for a Complex-One Dimensional Field", A. R. Bishop, S. Sarker, S. E. Trullinger, Physics Letters, 59A, 255, 1977.

"Possibility of a ϕ Particle Crystal in TTF-TCNQ", S. E. Trullinger and A. R. Bishop (preprint)

"Theory of the Low Temperature DC Conductivity of Weakly Pinned Fröhlich Charge-Density-Wave Condensates", S. E. Trullinger, A. R. Bishop, R. A. Guyer, J. A. Krumhansl (preprint).

"Dynamic Polarizability of the Sine-Gordon Soliton", A. R. Bishop, M. B. Fogel, S. E. Trullinger, Physics Letters, 59A, 2, 81, 1976.

"Solitons in a Coupled Linear Chain System", B. Horowitz and E. Domany, Physical Rev. Lett. 38, 14, 778, 1977.

"Numerical Simulation of Sine-Gordon Soliton Dynamics in Presence of Perturbations", J. Currie, S. Trullinger, A. R. Bishop, J. A. Krumhansl, preprint.

"Aspects of Exact Dynamics for General Solutions to the Sine-Gordon Equation", J. Currie, Physical Review A 16, 4, 1692, 1977.

"Solitary Structures in Nonlinear Fields", J. A. Krumhansl, Sanibel Conference, 1977.

"Formal Aspects of the Theory of the Scattering of Ultrasound by Flaws in Elastic Materials", E. Domany, J. E. Gubernatis, J. A. Krumhansl, J. of Applied Physics, 48, 2804, 1977.

"Thermodynamics of the Sine-Gordon Field", M. B. Fogel, P. L. Palmer, J. F. Currie, Physical Review A16, 796, 1977.

"Aspects of Exact Dynamics for General Solutions of the Sine-Gordon Equation with Applications to Domain Walls", J. F. Currie, Physical Review A16, 4, 1692, 1977.

"Quasistatic Approximation to the Scattering of Elastic Waves by Circular Crack", E. Domany, J. Krumhansl, S. Teitel (Submitted for Publication).

"A Model for Phase Transition in TTF-TCNQ", B. Horovitz and D. Mukamel, Solid State Comm. 23, 285, 1977.

"Nonlinear Modes in the Condensed Peierls Phase", B. Horovitz and J. A. Krumhansl,

"Interphase Solitons in ω Phase Systems and the Central Peak", B. Horovitz, J. L. Murray and J. A. Krumhansl, Submitted for publication.

"Peierls Instability and Superconductivity in quasi-one-dimensional conductors", B. Horovitz, Physical Review B16, 3943, 1977.

"On the Theory of the Phase Transition in the Two-Dimensional Planar Spin Model", Peter Young, to be published.

"On the Theory of Melting in Two Dimensions", Peter Young, preprint.