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Astrophysical Materials Science:

Theory

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Final Technical Report

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I. Introduction

Since the initial award of Grant NGR-33-010-188 in summer of 1972, the aim of the project "Astrophysical Materials Science: Theory" has been to develop analytic methods to better our understanding of common astrophysical materials particularly those subjected to extreme physical conditions. The program was administered in the past by the staff of the Lewis Research Center, National Aeronautics and Space Administration, Cleveland, Ohio. In October, 1978, the project was administered by N.A.S.A. Washington, reappearing under the same title as NSG-7487. Beginning December 31, 1981, the project was transferred for administrative purposes to NASA, Ames Laboratory, Moffett Field. The contract ended on December 1, 1983.

This document briefly summarizes the research discoveries and work carried out on these various contracts. Hydrogen and helium constitute by far the most abundant of the elements, and it is no accident that the research continues to be focused heavily on these elements in their condensed forms, both as pure substances and in mixtures. It will be seen below that the research has combined the fundamental with the pragmatic. The proper and complete understanding of materials of astrophysical interest requires a deep appreciation of their physical properties, especially when taken into the unusual ranges of extreme conditions. Fundamental theoretical condensed matter physics has played a very important part in the research to date, and will continue to be a dominant element in any research carried out in the future. The collaboration with the experimentalists at

Cornell (Professor Ruoff and his group) have also been exceedingly beneficial.

The research will now be summarized.

II. Research Synopsis

Attached to this document are three Appendices listing the cumulative publications of work supported by NASA under Grants NGR-33-010-188, NSG-7487, and NAG 2-159. Papers #1-13 give the background necessary to place the research supported by Grants NSG-7487 and NAG-2-159 in proper context. The themes developed in this work can be described briefly as follows.

Paper #1, on the ground state energies of simple metals, developed the method of structural expansions for use in determining the equation of state of metallic hydrogen (and indeed other metals) up to 4th order in perturbation theory. Previously, work in the Soviet Union and elsewhere had made predictions on the nature of the structure of metallic hydrogen based on lower perturbation theory. Paper #1 called this into question, at least for static lattices.

Paper #2 concerned itself with the nature of the deep interior of Jupiter, particularly with respect to the transport properties. We were able to calculate both the electrical and thermal transport properties of the planetary interior and hence comment on the origin of the Jovian magnetic field.

Paper #3 is devoted to a problem in molecular hydrogen, specifically the nature of the interaction between molecules at short range and the importance of multi-center terms in arriving at an adequate description of the thermodynamic functions of condensed molecular hydrogen.

Paper #4 returned to the subject of Paper #1 and took up the question of proton dynamics, again arriving at a method applicable to many metals. In accounting for the structural energies in a dynamic lattice, we also obtained a method for determining x-ray structure factors (particularly diffuse thermal scattering) which has been very useful.

Paper #5 addresses a problem raised in Paper #2, namely, are metallic hydrogen and metallic helium mutually soluble under the conditions prevailing in the deep interior of Jupiter? The results of the calculations presented in Paper #5 show fairly convincingly that almost complete phase separation is to be expected, and this has interesting consequences in the transport properties as a function of depth into the planet.

Paper #6 tackles a question emerging from Paper #4, namely, can the proton and electron degrees of freedom really be separated when dealing with the thermodynamic functions of hydrogen, or should they be treated as coupled systems? The latter is found to be the case, and the structural consequences are really quite important. Simple structures are favored by this approach, rather than the grossly anisotropic structures proposed by the Soviet groups.

Paper #7 continues the work of Paper #5, but continued into the domain of liquid rather than solid solutions of hydrogen and helium. The miscibility gap in the solid is found to persist in the liquid alloys unless the temperature gets exceedingly high. This has application in some stellar exteriors.

Paper #8 begins a study of molecular hydrogen and its band-structure and continues the work begun in Paper #3. The ultimate intent is the determination of the thermodynamic functions of the molecular phase, and then the estimation of the metallization pressure. The results of the

calculation introduce the notion that metallization by isostructural band-overlap may be a possibility.

Paper #9 deals with the quantum aspects of ground state defects in hydrogen and asks whether "quantum-defectons" can be present in metallic hydrogen crystals, and if so, whether they can coagulate into macroscopic voids whose surfaces may then be unstable to molecule formation. This prospect is ruled out by calculation: again a general method for dealing with systems other than hydrogen is introduced.

Paper #10 introduces a new idea: that the ground state of metallic hydrogen might be a quantum liquid. To obtain the ground state energy of such a system, it is then necessary to extend the theory of liquids somewhat and the paper deals with a method for obtaining the necessary distribution functions.

Paper #11 then takes up the idea of Paper #10 to calculate the ground state energy of a proposed liquid phase of metallic hydrogen and indeed finds that up to third order at least (in the electron-proton interaction) such a state is a very strong possibility. It also examines the likelihood of partially ordered magnetic phases, and notes that some of the ordering energies are quite characteristic of superconducting ordering energies.

Paper #12 extends the notions discussed in Paper #2 and discusses both the metallic and insulating form of hydrogen and helium in the context of models of the interior of Jupiter and Saturn.

Paper #13 is also concerned with Jupiter and Saturn, but from the standpoint of dynamic aspects, specifically convection and the influence on it of composition gradients in the mixture of hydrogen and helium.

III. Research 1978-81

Section II gives the background to the following more recent developments:

Paper #14 introduces a new way of describing dense molecular and dense metallic hydrogen from a common density functional framework. Since the same theoretical picture is used in both phases, systematic errors are eliminated. Metallization pressures in the neighborhood of 1.8 Mbar are predicted.

Paper #15 treats a theory of the liquid state applicable to insulating systems and metallic systems (for instance, liquid metallic hydrogen in the classical regime). It introduces a powerful reinterpretation of what is known as the reference hypernetted chain model (RHNC). In particular, it shows that all classical simple liquids are, to a high degree, universal when viewed in terms of the behavior of their bridge functions.

Paper #16 extends some of the ideas of universality (Paper #15) and gives an iterative argument establishing the insensitivity of the bridge-function to the choice of pair potential.

Paper #17 extends the ideas of Papers #16 and #17 even further to the interesting class of dense fluids characterized by very soft pair potentials. The high density classical plasma (e.g., hydrogen) is a case in point to which this theory can be applied.

Paper #18 deals with a dense one-component plasma but in a new context: the plasma confined to a two-dimensional surface. It is a simulation study in which the aim is to examine the thermodynamic functions, correlation functions, and ordering.

Paper #19 examines the role of the pair potential in a liquid metal in determining the details of the static structure. Normally the pair

potential is adequately represented in pseudopotential theory as a screened Coulomb interaction between ions. For certain systems, however, the fluctuating dipole contributions (dynamically screened by the electron gas) can lead to important corrections having noticeable structural consequences. The effect is present, in principle, in the light elements at high density.

Paper #20 extends the Monte-Carlo simulation methods developed in Paper #18 to the three-dimensional context. Specifically it treats the case of high density metallic hydrogen and comes to the interesting conclusion that over a certain density range the system may prefer to be a liquid metal at T = 0. This would be a new state of matter.

Paper #21 takes up this idea (a zero temperature liquid metal) and examines the physical properties of such a novel quantum-liquid. The paper generalizes two-component Fermi-liquid theory to the case of two components (electrons and protons).

Paper #22 begins to tackle the problem of the melting of hydrogen (in the density range where it is a solid at T = 0) by developing a hard-sphere crystal theory which largely parallels in intent the hard sphere liquid theory so successfully used in the treatment of classical liquids. The idea is to use a hard-sphere solid as a basis for perturbation treatments of real dynamic crystals.

Paper #23 is a discussion of possible ordered phases of liquid states of metallic hydrogen and deuterium near T = 0. It includes superconductivity and superfluidity. Again, a superconducting liquid metal would be a new state of matter.

Paper #24 extends the method introduced in Paper #14 to include a discussion of proton dynamics in the destruction of the paired state as pressure increases. It has direct relevance to two measurements of Raman

scattering from ultra-pressure hydrogen, one of which it supports and the other it does not.

Paper #25 applies some of the ideas of Papers #15-17 to the case of inhomogeneous fluids, for example, the surface of a classical fluid, or the boundary layer between a classical fluid and a container.

Paper #26 further extends the discussion presented in Paper #21 on the Fermi liquid properties of two-component Fermion systems. In particular, it presents stability criteria for these systems which must be obeyed if the fluid is to remain 'normal' (i.e., no pairing).

Paper #27 presents the necessary theory for a liquid superconducting state. It begins with the Eliashberg equations and because of the translational and rotational symmetry of a liquid (not present, of course, in a crystalline solid) can reduce them to manageable forms. The predicted transition temperatures for superconductivity are still very high.

IV. Research 1981-83

For the background on this phase of our research, the reader is referred to sections II and III, above. The papers now to be described were supported by the NASA-Ames Agreement (NAG 2-159). Appendix III lists the appropriate citations.

Paper #28 reviews the progress in elucidating the theoretical issues raised by the prospects of two new quantum liquids namely liquid metallic deuterium and liquid metallic hydrogen. Both would be novel states of matter.

Paper #29 gives a rather complete theory of the transport properties of a two component Fermi liquid starting with the generalized Landau-Silin-Boltzmann equations. It's shown that the transport properties of liquid

metallic hydrogen are dramatically different from those of its crystalline counterpart.

Paper #30 addresses a variational approach to the groundstate energy of dense molecular and metallic hydrogen within the spin-restricted Hartree-Fock approximation. It is explicitly demonstrated that bond-separations within molecules change rapidly at the onset of the metal-insulator transition.

Paper #31 proves an interesting cusp theorem that relates the zero-separation value and slope of two particle positional correlation functions in quantum many-body systems with Coulombic interactions. The theorem was applied to atomic-orbital based models of both molecular hydrogen and metallic hydrogen.

Paper #32 examined the behavior of the critical fields of liquid superconducting metallic hydrogen. The system is precicted at certain densities to pass from dirty to clean and from type-II to type-I behavior as temperature is lowered. The change in type is associated with a strong temperature dependence of the basic electron transport time.

Paper #33 addresses two possible types of pairing involving the protons in a low-temperature liquid phase of metallic hydrogen. One is the many-body generalization of the basic electron-proton pairing familiar in the atomic context. The other is a proton-proton pairing analogous to that occurring in the ordered phases of liquid He^3.

Paper #34 further examines the energetics of some liquid-like states of dense hydrogen, and specifically addresses the difficulties of obtaining accurate estimates when using many-body perturbation theory.

Paper #35 comments on a derivation of acoustic plasma modes in two component Fermi liquids which appeared in the literature but which was

easily shown to be incorrect. Metallic hydrogen is an example of such a system and which has but a single longitudinal acoustic mode (in contrast to three such modes, as was recently claimed).

V. Conclusions

Metallic hydrogen, metallic deuterium, and metallic helium have considerable importance in the content of planetary interiors and stellar interiors. In such surroundings the systems are undoubtedly in the classical regime, and in this range of densities and temperatures their properties are extremely interesting. Even more fascinating, however, are their properties in the quantum regime. It is not yet established firmly that metallic hydrogen and deuterium can exist as liquids at low temperatures and at certain densities. However, the prospect looks very probable and, if true, the range of predicted properties for metallic hydrogen will greatly exceed the initial expectations. Thus, the highly quantum aspects of high density hydrogen and helium will remain a source of interesting physics and astrophysics for some time to come.

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Appendix I
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CUMULATIVE PUBLICATIONS: NAG-2-159
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