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Radiation Laboratory

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JULY-SEPTEMBER 1964

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FOREWORD

The Physics Department Progress Report has been initiated to provide a greater degree of communication among the divisions, projects, and groups of this Laboratory and for the benefit of the scientific community at large.

This periodic report will incorporate into one comprehensive entity those investigations in the fields of experimental and theoretical physics which immediately support the Laboratory programs on a long-term basis. Its object will be to show the status of unclassified projects and programs conducted within the Physics Department, and to provide a continuous record of the progress made in the field of physics at this Laboratory.

Each report, consisting of summaries of completed work, preliminary results and interim progress, will cover a period of four months. In order to facilitate referral, each article will have a reference to the original paper which has been published or which has been submitted for publication.

NUCLEAR AND ATOMIC PHYSICS

Theoretical

Nuclear Structure

In recent work¹ we have shown that by using a variational type of wave function flexible enough to take account of the short- and long-range correlations between all pairs of particles we can get very reliable estimates to the eigenvalue of a few-body system. We have tested this type of trial function extensively by calculating both the upper and lower bounds to the eigenvalue for the three- and four-body systems with the result that in both the core and asymptotic regions our trial function is quite adequate. Using the hard-core nucleon-nucleon potential found by Ohmura *et al.*,² which fits the low-energy two-body data, and using our type of trial function, we have found³ that only for a core radius between 0.35 and 0.50 F could reasonable agreement with the experimental binding energies, the Coulomb energy, and the r. m. s. radii of these systems be obtained. This is of interest since the phenomenological hard-core nucleon-nucleon potentials obtained from analyses of the two-nucleon scattering experiments all have a core radius lying within this range.

With this two-body hard-core potential and our type of trial function, which explains in a consistent way the two-, three-, and four-body systems, we have been investigating the Λ -N and Λ - Λ interaction. In our recent studies of the hypertriton⁴ and the other S-shell hypernuclei with $A \leq 5$ (Ref. 5) we have determined the triplet and singlet depth for a central Λ -nucleon potential of hard-core radius 0.4 F and an attractive part of exponential shape, with an intrinsic range for the Λ -N interaction which corresponds to the two-pion exchange. The results show the singlet interaction to be stronger than the triplet.

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¹Y. C. Tang, R. C. Herndon, and E. W. Schmid, Phys. Rev. 134, B743 (1964); Y. C. Tang, E. W. Schmid, and R. C. Herndon, BNL 8293 (1964).

²T. Kikuta, M. Morita, and M. Yamada, Prog. Theor. Phys. 15, 222 (1956); T. Ohmura, Prog. Theor. Phys. 22, 34 (1959).

³Y. C. Tang, E. W. Schmid, and R. C. Herndon, BNL 8293 (1964).

⁴R. C. Herndon, Y. C. Tang, and E. W. Schmid, Nuovo Cimento 33, 259 (1964).

⁵R. C. Herndon, Y. C. Tang, and E. W. Schmid, UCRL 12037 (1964).

The strength of the Λ -nucleon interaction found by us strongly indicates that the hyperdeuteron is not a bound system, though the strength is large enough so that we cannot rule out the possibility of the existence of a bound excited state in ΛH^4 and ΛHe^5 in the neighborhood of 0.35 MeV. We have, in addition, calculated the binding energy of a particle in nuclear matter and the Λ -nucleon scattering cross sections. In both cases fair agreement with experimental data has been obtained. These results, combined with the fact that with this potential we can obtain the observed S-shell hypernuclear binding energies, indicate that there is no need to use more complicated potentials to explain the existing phenomena. At present, the use of a two-body spin-dependent central potential with hard core seems to be entirely sufficient.

As a next step it seems desirable to look at the P-shell hypernuclei with ΛLi^7 as a good choice to start with, since the core nucleus Li^6 has already been examined with a hard-core nucleon-nucleon potential similar to ours, and very satisfactory results for its binding energy and r. m. s. radius were obtained.⁶ The calculation on such a large system is, of course, difficult, but it can still be handled with the Monte Carlo technique we have used previously. These results concerning P-shell hypernuclei should give us more information about the Λ -nucleon interaction than is known now.

We are also investigating the strength of the Λ - Λ interaction by using the observed data on the double hyperfragment $\Lambda\Lambda\text{Be}^{10}$ found by Danysz et al.⁷ By first using a three-body model of $\Lambda + \Lambda + \text{Be}^8$ (g. s.) and a Λ - Λ potential with hard core and of exponential shape, we found the potential depth to be $V_{\Lambda\Lambda} = -1056 \pm 38$ MeV and a scattering length and well depth parameter of

$$a_{\Lambda\Lambda} = - (1.93^{+0.51}_{-0.38}) \text{ F}$$

and

$$s_{\Lambda\Lambda} = 0.817 \pm 0.029,$$

respectively.⁸ With this value of $V_{\Lambda\Lambda}$ we also computed the separation energy $B_{\Lambda\Lambda}$ of $\Lambda\Lambda\text{He}^6$ and obtained the result of 11.08 ± 0.11 MeV, which is very

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⁶E. W. Schmid, Y. C. Tang, and K. Wildermuth, Phys. Letters 7, 263 (1963).

⁷M. Danysz et al., Phys. Rev. Letters 11, 29 (1963).

⁸Y. C. Tang, R. C. Herndon, and E. W. Schmid, Phys. Letters 10, 358 (1964).

close to the value of 11.2 MeV obtained by Dalitz and Rajasekaran.⁹ In the three-body calculation of $\Lambda\Lambda\text{Be}^{10}$, distortion of the Be^8 core nucleus was not taken into account. To consider this effect on the value of $V_{\Lambda\Lambda}$ we are just in the process of finishing a calculation where we have treated $\Lambda\Lambda\text{Be}^{10}$ as $2\alpha + 2\Lambda$ and the preliminary results do, indeed, show that the Be^8 core is compressed slightly. The results of this work will be published shortly.

R. C. Herndon

Correction to the Potential in Born Approximation Arising From Direct Channel Strips

The study of the π - π strong interaction based on the Mandelstam Representation and the N/D method has been pursued by many authors.¹⁰ The original studies were made without Regge continuation, but more recent research is aimed at understanding the π - π problem based on analytic continuation into the complex angular momentum plane.¹¹ The basic idea in Refs. 10 and 11 is to generate the π - π scattering amplitude in the state (ℓ, I) by constructing an N/D solution with a given driving force fed in through N. The driving force is assumed to be saturated by keeping only intermediate exchanges of poles in crossed reactions that can communicate with the initial and final 2- π states. This is essentially the "strip approximation"¹² to the driving force, and the potential may therefore be thought of as the strips of the double spectral regions corresponding to the crossed reactions. Chew¹³ has pointed out that the direct channel strips must also contribute to the driving force, but this correction has never been included in a practical calculation of π - π dynamics. The purpose of this study has been to write down a numerically manageable formula for estimating this effect.

The π - π partial wave amplitude has been studied in the one-channel approximation for the states $\ell = 1, I = 1$, and $\ell = 2, I = 0$. The Born approximation to the force operating in the direct channel was assumed to be

⁹R. H. Dalitz and G. Rajasekaran, Nucl. Phys. 50, 450 (1964).

¹⁰G. F. Chew and S. Mandelstam, Phys. Rev. 119, 467 (1960); L. Balázs, Phys. Rev. 128, 1939 (1962) and references given therein.

¹¹G. F. Chew and V. L. Teplitz — private communication.

¹²G. F. Chew and S. Frautschi, Phys. Rev. Letters 7, 394 (1961).

¹³G. F. Chew — private communication.

saturated by ρ -exchange in the crossed reactions for both states. This amounts to a "strip approximation" to the force. However, the direct channel strips must also contribute to the potential, and it is important to ask how significant this correction is for π - π scattering. It has been found that the effect produces an additional attractive force in both states and that it is not overwhelming in either state and may very well be negligible.

M. Der Sarkissian*
(UCRL-12025-T)

Reciprocal Bootstrap Mechanism

Self-consistent bootstrap calculations¹⁴ of the ρ meson ($\ell = 1$, π - π resonance) as a pure elastic resonance in the π - π system have generally resulted in too low a ρ mass and too large a width for ρ decay. Attempts to improve the results by including other channels, such as π - ω or K - $\bar{K}$, while still keeping ρ exchange as the dominant force mechanism, have improved the mass somewhat but still require much too large a self-consistent width.¹⁵ The present work is a departure from previous models of the ρ and considers a reciprocal bootstrap mechanism between the ρ and a $j = 2$, $\ell = 1$ resonance in the π - ω system identified as the B meson.¹⁶ In this model the exchange of the B in the π - ω system provides a force which is strong enough to bind the π and ω forming the ρ meson as a π - ω bound state. It decays into two pions but has its dynamical origin in the π - ω system.

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*Lawrence Radiation Laboratory Postdoctoral Fellow.

¹⁴F. Zachariasen, Phys. Rev. Letters 7, 112, 268 (E) (1961); D. Y. Wong, Phys. Rev. 126, 1220 (1962); L. Balazs, Phys. Rev. 129, 872 (1963).

¹⁵F. Zachariasen and C. Zemach, Phys. Rev. 128, 849 (1962); J. R. Fulco, G. L. Shaw, D. Y. Wong, Phys. Rev. (to be published).

¹⁶M. Abolins, R. L. Lander, W. A. W. Melhop, Nguyen-Huu Xuong, and P. M. Yager, Phys. Rev. Letters 11, 389 (1963); L. Bondar, E. Keppel, G. Kranes, W. P. Dodd, B. Tallini, G. Wolf, I. Butterworth, F. I. Campayno, M. Ibbotson, N. N. Bisevas, I. Derado, D. Luers, and N. Schmitz, Phys. Rev. Letters 5, 209 (1963).

The model used is an extension of the static π - ω model used by R. F. Peierls¹⁷ to predict the properties of the B meson as due to the attractive force resulting from ρ exchange. A natural extension of this model as first proposed by Chew¹⁸ for the reciprocal bootstrap relationship of the N and N^* in the π -N system then establishes a similar relationship between the ρ and B in the π - ω system. The N/D method of solution of the π - ω static dispersion relations is used and the zero width and effective range approximations lead to simple conditions on the crossing matrix to guarantee self-consistency. These conditions are then shown to hold for the ρ and B reciprocal bootstrap. By self-consistency is meant that the $\rho(B)$ meson whose exchange produces the B(ρ) meson has identical properties to the $\rho(B)$ meson produced by B(ρ) exchange. Further calculations show that the relative magnitudes of the forces are such that if the Peierls model of the B meson is correct, then the B exchange force is indeed strong enough to bind the π - ω system forming the ρ meson. The calculated width of the B is in reasonable agreement with experiment, while the estimated ρ mass is 870 MeV. This is higher than experiment (760 MeV) but this calculation should be expected to give too high a ρ mass because it does not include the π - π channel, where the force is known to be attractive in the $\ell = 1$ state. The width of the ρ is undetermined in this calculation but the puzzle of how the ρ could have a relatively narrowed width at a relatively high π - π energy is solved if it is predominantly a π - ω bound state as proposed here.

J. Franklin

Least-Squares Analysis and Significance Tests for a Set of Functions of Discrete Abscissae

The problem of least-squares fitting $\underline{m}$ sets of $\underline{n}$ experimental data points, occurring at $\underline{m}$ abscissae, by means of $\underline{n}$ curves, has been investigated in the case when the values of the data are distributed randomly with uniform probability between two fixed limits. The problem is relevant to a

¹⁷R. F. Peierls, Phys. Rev. Letters 12, 50, 119 (E) (1964). Peierls' model has been extended in a relativistic treatment by R. K. Kuo, Phys. Rev. Letters, 12, 465 (1964).

¹⁸G. F. Chew, Phys. Rev. Letters 9, 233 (1962).

test of the Regge pole hypothesis of elementary particles,¹⁹ but the present paucity of data does not permit an application of the results of this paper, and hence no statement can be made whether the Regge classification of particles is meaningful or not..

The derived expression for the probability density function of the chi-square distribution for a given assignment may be combined with the expression which gives the probability density function of the chi-square. The latter is applicable in situations where there are several ways of fitting the data due to a multiplicity of data points and of fitting curve. This enables one to predict the expected chi-square distribution by fitting m sets of n experimental data at m abscissae, if the distribution of these data points are random with uniform probability within a finite range. The constraint of a finite range for the data points might turn out to be useful in actual applications for several reasons. First, we can in this way incorporate into our analysis the requirement that the trajectories be limited by the so-called Pomeranchuk trajectory. But even if one does not want to use such a specific assumption, it might be useful to limit the range of data points by other, more general arguments. In particular, one can assume that if strong interaction forces have a range of the order of a fermi, and if all elementary particles can be looked upon as, in some sense, put together out of some other particles, the angular momentum state in which such a "resonance" can occur at a given energy is limited by the usual impact parameter arguments. This would automatically impose an upper limit on the spin of an elementary particle with a given mass, and this upper limit would increase with increasing energy, in qualitative agreement with the predictions of the RPH. Such a limit should therefore be incorporated into a future analysis utilizing the results of this work, so that the more specific predictions of the RPH could be tested in themselves.

In the above considerations we assumed that the individual data points are randomly distributed with uniform probability over a finite range. This is the distribution one would expect if there were no correlation between the Regge classification and physical reality. If the Regge classification is, however, meaningful, one should rather assume a Gaussian distribution about

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¹⁹G. F. Chew, M. Gell-Mann, and A. Rosenfeld, Scientific American 210, No. 2, 74, (1964).

some "true" value. Under such an assumption, part of the calculation could be redone in a way very similar to the present method, and such a calculation can in fact be expected to be much simpler than the present one.

M. Moravcsik and H. D. I. Abarbanel^{*}
(UCRL-12071-T)

Pion-Proton Phase-Shift Analyses

Other laboratories have recently been doing pion-nucleon phase-shift analyses up to 700 MeV.^{20, 21} We have compared their results with ours²² in a 300-700 MeV analysis using some new data and using $\text{Re } f^{\pm}(0)$ as data.²³ We obtained the best fit to the data with the London solution.²⁰ This solution differs from our previous solution²² in the following important ways:

S_{11} states: The phase shift peaks (47°) at 600 MeV and drops down to $\sim 0^\circ$ at 700 MeV. Ours continued past 50° .

P_{11} states: The phase shift peaks (100°) at 600 MeV and drops to 60° at 700 MeV. Ours continued to 120° at 700 MeV.

There are also other minor differences.

We have closely examined several 0-350 MeV solutions that we have obtained from widely varying input. The solutions differ very little in their predictions of all possible observables. Experiments to distinguish among the solutions are probably impossible to do with present technology. This work will be published soon.

Presently we are trying to extend the analysis to 1100 MeV in a 700-1100 MeV analysis. Some difficulty has been encountered in finding a solution that agrees with the 300-700 MeV best solution at 700 MeV.

L. D. Roper

Possible Electromagnetically Induced Muonium-Antimuonium Conversion

The possibility of the existence of an electromagnetically induced transition between muonium and antimuonium has been examined. An

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^{*}Department of Physics, Princeton University, Princeton, New Jersey.

²⁰P. Auvil, C. Lovelace, A. Donnachie and A. T. Lea, Physics Letters 12, 76 (1964).

²¹B. H. Branden, R. G. Moorhouse, and P. J. O'Donnell, NIRL/R/70 (1964).

²²L. D. Roper and R. M. Wright, UCRL 7846 (1964).

²³G. Höhler, G. Ebel, and J. Giesecke, Karlsruhe preprint (1964).

experiment has been suggested involving the formation of muonium by the injection of positive muons into a helium-filled resonant cavity, which is excited at a frequency corresponding to the difference in interaction energy between muonium and helium on the one hand, and that between antimuonium and helium on the other. The sign of antimuonium formation is the observation of the fast negatons from μ^- decay. The dependence of the number of these on which of various cavity modes is excited gives information on the relative intrinsic parity of muonium and antimuonium. If this turns out to be odd then this measurement, when combined with the usual relation for the product of the intrinsic parities of a Dirac particle and its antiparticle, would determine the relative intrinsic parity of the muon and electron to be imaginary. The conservation of parity in electromagnetic phenomena and the absence of electromagnetic μ -e transitions would then both find their natural explanation in the single previously suggested assumption²⁴ that the observation of electromagnetic phenomena must be compatible with invariance under space inversion.

M. J. Moravcsik and R. K. Spitzer
(UCRL-12009-T)

K_1^0 Regeneration by Magnetic Field and Apparent CP Violation

The results of two recent experiments^{25, 26} indicate the presence of 2π decay modes of the neutral K meson at distances corresponding to very many K_1^0 decay lengths from the target. Since the experimental arrangements exclude the possibility that these were decays of K_1^0 's regenerated by matter, these results have been interpreted^{26, 27} as evidence for 2π decays of the K_2^0 .

The observed 2π decays are predicted on the basis of theoretical proposals^{27, 28} suggested some time ago, and that relatively slight modifications

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²⁴R. Spitzer, Nucl. Phys. 51, 553 (1964).

²⁵J. H. Christenson, J. W. Cronin, V. L. Fitch, and R. Turlay, Phys. Rev. Letters 13, 138 (1964).

²⁶A. Abashian, R. J. Abrams, D. W. Carpenter, G. P. Fisher, B. M. K. Nefkens, and J. H. Smith, Phys. Rev. Letters, 13, 243 (1964).

²⁷R. Spitzer, Nucl. Phys. 21, 681 (1961).

²⁸R. Spitzer, Nucl. Phys. 47, 367 (1963).

in the experimental arrangements described in Refs. 25, 26 would be sufficient to test the relevance of these proposals. The interpretation of these events suggested here does not invoke CP violation and is quite different from that given in Refs. 25 and 26.

The mechanism derived from the proposed interaction^{27, 28} to account for the above results is K_1^0 regeneration by the component $H_{||} = \underline{p} \cdot \underline{H}/p$ of an external magnetic field parallel to the K momentum $\underline{p}$. The observed 2π decays would then simply be the regular mode of the regenerated K_1^0 . It appears from the described experimental arrangements that in both experiments such a magnetic field is present close to the decay position.

The strength of the proposed interaction is an unknown parameter that must be determined from experiment so it is not possible to predict the magnitude of the effects. It should be relatively easy, however, to test whether the interaction can account for the observed 2π decays; namely by changing the value of $H_{||}$ within the sensitive region of the experimental set-up.

In conclusion it should be noted that if the proposed interaction is present in sufficient strength, the neutral K meson could very well turn out to be an extremely useful probe of electromagnetic fields in media in which the use of electrically charged particles for this purpose is not practical.

R. K. Spitzer
(UCRL-12068-T)

The LSZ Formalism in the Lee Model

In the formal investigation of field theory, the axiomatic approach of Lehmann, Symanzik, and Zimmerman²⁹ (LSZ) has played a major role. The LSZ asymptotic condition, expressing the weak convergence of the Heisenberg fields to the "in" and "out" fields, allows an interpretation of field theory in terms of physical particles. Using this condition, a reduction formula can be obtained relating the S-matrix elements for processes involving the physical particles to the " τ -functions."³⁰ A coupled set of integro-differential

²⁹H. Lehmann, K. Symanzik, and W. Zimmerman, Nuovo Cimento 1, 205 (1955).

³⁰The τ -functions are the vacuum expectation values of time-ordered products of the Heisenberg fields.

equations can then be derived for these functions, from the field equations and commutation relations.³¹

In this paper, the LSZ formalism is applied to a solvable field theory, the Lee model.³² This model describes the S-wave interaction between two fermions, the V and N particles, and relativistic, spin-zero bosons, the θ particles. Spin and recoil are neglected for the fermions. The interaction is $V \leftrightarrow N + \theta$.

First, it is shown that the LSZ asymptotic conditions on the V, N, and θ fields are equivalent to the statement that scattering states can be constructed in the usual manner. Then the reduction formula is derived, giving the relation between the Fourier transforms of the τ -functions, when evaluated on the energy shell, and the conventional T-matrix elements.

We then consider the lowest nontrivial sector of the model, in which there are V particle renormalization and N- θ scattering. The equations for the appropriate τ -functions are written down and solved algebraically, by transforming into momentum space. By studying the analytic structure of the V propagator, the renormalization constants are obtained. The S-matrix element for N- θ scattering is then computed.

In the literature, this sector has been solved both by solving the eigenvalue equations³² and by using a dispersion treatment.³³ It is found that the τ -function approach elucidates the basic structure of the model in the most natural way, giving rise to considerable mathematical simplification.

M. S. Maxon

Reaction Threshold Tabulations

A tabulation of thresholds for reactions induced by neutrons, protons, deuterons, tritons, He^3 , and He^4 , in the laboratory system, has been derived from the tabulation of binding energies given by König et al.,³⁴ and the

³¹P. T. Matthews and A. Salam, Proc. Roy. Soc. (London) A221, 128 (1953).

³²T. D. Lee, Phys. Rev. 95, 1329 (1954). G. Kallen and W. Puli, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 30, No. 7 (1955).

³³M. L. Goldberger and S. B. Treiman, Phys. Rev. 113, 1663 (1959). P. DeCelles and G. Feldman, Nucl. Phys. 14, 517 (1960).

³⁴K. König, H. J. Kuntze, and H. J. Kuntze, Nucl. Phys. 14, 517 (1960).

references contained therein. This tabulation is primarily for those who need a ready reference.

The definition of the threshold used here is: the minimum kinetic energy of an impinging particle (in the laboratory system) such that the reaction is energetically possible. In view of this definition, all reactions having positive Q value have a threshold of zero. Those reactions having a negative Q value have a threshold of $-[(A + M)/A] Q$ (where M is the rest mass of the incident particle). For those reactions for which the binding energy of the residual nucleus is not given in König et al.,³⁴ dashes are entered in the table. This tabulation has been published in UCRL reports 14001 through 14006.

R. J. Howerton, W. J. Cahill,
D. L. Braff, N. J. Chazan

Experimental

Epithermal Fission Cross Section of Am^{241}

The corona-type spark chamber has been adapted for detection of fission fragments in the presence of intense alpha activity to allow measurements on large samples of highly alpha active nuclei. A detector containing 200 mg of Am^{241} was used for a study of the fission cross section in the epithermal region by the time-of-flight method. The 30-MeV Livermore electron linac was used as the pulsed neutron source. The results are given in Figs. 1 and 2. All of the eleven resonances observed below 6.5 eV in the total cross section³⁵ were observed in the measurements except for the small resonance at 4.40 eV. A small resonance at 1.68 eV which appears to be weakly indicated in the total cross section also was observed in the fission measurements. The three lowest energy resonances were analyzed by single-level shape analysis. The resulting parameters are in good agreement with earlier work on these resonances.³⁶ Using the average capture width thus

³⁴L. A. König, J. H. E. Mattauch, A. H. Wapstra, Nucl. Phys. 31, 18 (1962).

³⁵J. A. Harvey, R. C. Block, and G. G. Slaughter, Bull. Am. Phys. Soc., Ser. II, 4, 34 (1959).

³⁶B. R. Leonard, Jr., Nuclear Physics Research Quarterly Report HW-59126 (1959) p. 3.

Fig. 1. Epithermal fission cross section of Am^{241} between 0.03 and 1.5 eV.

Fig. 2. Epithermal fission cross section of Am^{241} between 1.5 and 80 eV.

obtained, it is possible to determine values of Γ_f for the remaining resonances by area analysis. The value of $\langle \Gamma_f/D \rangle$ is in good agreement with that expected from the shape of the fast neutron fission threshold. The effective number of fission channels determined from the distribution of fission widths is 2.8 ± 0.6 . For the $5/2^-$ target, 3^- and 4^- spin states are excited by the addition of s-wave neutrons. Since all resonances in the total cross section were seen in the fission cross section, the fission channels for the two spin states are probably open to about the same degree. According to the collective model, the lowest intrinsic states in the compound nucleus Am^{242} are the 1^- and 5^- states. Vibrational states and other intrinsic states would be expected at a considerably higher energy. According to the Bohr³⁷ model for fission, slow neutron fission therefore should proceed almost exclusively through the 3^- and 4^- members of the $K = 1^-$ rotational band. Since the 3^- and 4^- rotational states lie quite close together in energy, both channels should be open nearly to the same degree. This is consistent both with the observation of the same resonances in the total and fission cross section and with the number of effective channels derived from the fission width distribution.

C. D. Bowman, M. S. Coops,
G. F. Auchampaugh, and S. C. Fultz
(UCRL-7971)

The Angular Distribution and Polarization of Neutrons from the $\text{Be}^9(p, n_0)\text{B}^9$ and $\text{B}^{11}(p, n_0)\text{C}^{11}$ Reactions

The angular distribution of neutrons from the $\text{Be}^9(p, n_0)\text{B}^9$ reaction (Fig. 3) has been measured for the proton energies between 3.5 and 10.9 MeV and from the $\text{B}^{11}(p, n_0)\text{C}^{11}$ reaction (Fig. 4) at 7.1 and 8.2 MeV over the angular range 0 to 150° . The polarization of the neutrons from the two reactions was measured for proton energies from 7 to 11 MeV and neutron emission angles between 0 and 80° . Both experiments employed the Livermore neutron time-of-flight facility. The experimental method and apparatus employed in measuring the angular distribution and polarization are

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³⁷A. Bohr, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy 2, 151, United Nations, New York (1956).

Fig. 3. Angular distribution of ground-state neutrons from proton bombardment of beryllium.

described in detail elsewhere.^{38, 39} The measured angular distributions for the $\text{Be}^9(p, n_0)$ and $\text{B}^{11}(p, n_0)$ reactions are displayed in Figs. 3 and 4. The $\text{B}^{11}(p, n_0)$ angular distributions were measured at only two energies in order to provide an absolute normalization for the relative measurements of Overley and Borchers.⁴⁰ The $\text{Be}^9(p, n_0)$ angular distribution shapes (Fig. 3) are relatively insensitive to bombarding energy above 7.1 MeV while that for $\text{B}^{11}(p, n_0)$ ⁴⁴ fluctuates rapidly over the same proton energy interval. The same qualitative behavior is observed in comparing the polarizations from the two reactions (Figs. 5 and 6); the angular dependence of the polarization is a more sensitive function of bombarding energy in the case of the $\text{B}^{11}(p, n_0)$ reaction. These observations on the $\text{Be}^9(p, n_0)$ and $\text{B}^{11}(p, n_0)$ reaction pair

³⁸C. Wong, J. D. Anderson, S. D. Bloom, J. W. McClure, and B. D. Walker, Phys. Rev. 123, 598 (1961).

³⁹B. D. Walker, Ph.D. Thesis, LRL, Livermore, UCRL-7676 (1964).

⁴⁰J. C. Overley and R. R. Borchers (to be published in Nuclear Physics).

Fig. 4. Angular distribution of ground-state neutrons from proton bombardment of boron.

Fig. 5. Polarization of ground-state neutrons from proton bombardment of beryllium.

Fig. 6. Polarization of ground-state neutrons from proton bombardment of boron.

are not in accord with the twin reaction hypothesis of Bloom et al.⁴¹

B. D. Walker, J. D. Anderson,
J. W. McClure, and C. Wong
(UCRL-12019)

Beta Decay Asymmetry and Nuclear Magnetic Moment of Argon-35

In allowed beta decay, the angular distribution of electrons emitted from polarized nuclei is given by⁴²

$$W(\theta) = 1 + \frac{\langle m_I \rangle}{I} A \frac{v}{c} \cos \theta, \quad (1)$$

where I is the spin of the parent nucleus, v is the electron velocity, c is the velocity of light, and θ is the angle between the direction of electron emission and the spin quantization axis. We have measured the beta decay asymmetry parameter A for argon-35 and have determined the nuclear magnetic moment of argon-35 by observing the change in $W(\theta)$ which occurs when nuclear polarization is altered by resonance reorientation. The results are as follows:

$$A(\text{Ar}^{35}) = +0.16 \pm 0.04$$

and

$$\mu(\text{Ar}^{35}) = +0.632 \pm 0.002 \text{ nm.}$$

The experimental method is the same as that used previously for a similar experiment on neon-19.^{43, 44}

Argon-35 was produced by the reaction $\text{Cl}^{35}(p, n)\text{Ar}^{35}$ at the 90-inch cyclotron. Polarized atoms were obtained by passing an atomic beam of argon-35 through an inhomogeneous magnetic field and collecting one of the spatially separated polarized beams in a deflector bulb. Polarized atoms decay while trapped in the bulb. The decay electrons pass through thin

⁴¹S. D. Bloom, N. K. Glendenning, and S. A. Moszkowski, Phys. Rev. Letters 3, 98 (1959).

⁴²E. J. Konopinski, Ann. Rev. Nucl. Sci. 9, 104 (1959).

⁴³E. D. Commins and D. A. Dobson, Phys. Rev. Letters 10, 347 (1963).

⁴⁴D. A. Dobson, Lawrence Radiation Laboratory, Berkeley, Rept. UCRL-11169 and thesis, University of California, Berkeley (1964).

windows in the bulk and are counted to establish the asymmetry parameter A.

The Gamow-Teller matrix element for the superallowed beta decay of argon-35 was determined from A:

$$\langle \sigma \rangle = +0.10 \pm 0.05.$$

This result is consistent with the measured ft-value⁴⁵ and electron-neutrino correlation coefficient⁴⁶ which set upper limits on $\langle \sigma \rangle$. The results for $\langle \sigma \rangle$ and μ are in reasonable agreement with predictions based on a nuclear structure calculation using Nilsson's rotational model.⁴⁷

F. P. Calaprice, E. D. Commins* and D. A. Dobson
(UCRL-7999)

Magnetic Studies at the Livermore Pool Type Reactor

Measurements of the magnetic susceptibility and electrical resistivity of a single crystal of NiS have been made recently. Previous neutron diffraction powder studies⁴⁸ of NiS indicated the existence of an unusual first-order magnetic transition at 263° K in the NiAs-type crystal form of this compound. The neutron diffraction results were interpreted in terms of an antiferromagnetic structure appearing abruptly at 263° K on cooling. A further study⁴⁹ of the diffuse neutron scattering above and below the transition temperature suggested that there are no localized magnetic moments associated with the nickel atoms above the transition. These results imply that there are changes occurring in the electronic structure of this compound at the 263° K transition. The recent resistivity and susceptibility measurements were made to gain further insight into the nature of the transition.

*Physics Department, University of California, Berkeley, California.

⁴⁵O. C. Kistner, A. Schwarzschild, and B. M. Rustad, Phys. Rev. 104, 154 (1956).

⁴⁶W. B. Hermannsfeldt, R. L. Burman, P. Stahelin, J. S. Allen, and T. H. Braid, Bull. Am. Phys. Soc. 4, 77 (1959).

⁴⁷S. F. Nilsson, Kgl. Danske Videnskab. Selskab Mat.-Fys. Medd. 29, No. 16 (1955).

⁴⁸J. T. Sparks and T. Komoto, J. Appl. Phys. 34, 1191 (1963).

⁴⁹J. T. Sparks and T. Komoto, J. Phys. Radium (in press) (UCRL-7336-T).

The temperature independence and magnitude ($50 \times 10^{-6} \Omega\text{-cm}$) of the electrical resistivity parallel to the c-axis of the crystal above 263°K shows that this compound is metallic in behavior above the transition. On cooling, the resistivity increases abruptly at 263°K to $3800 \times 10^{-6} \Omega\text{-cm}$ and shows semiconducting behavior on further cooling. The metallic behavior above 263°K is consistent with the neutron results above 263°K , indicating the lack of localized moments. The semiconducting behavior below 263°K is also consistent with the neutron results, which indicated the existence of an antiferromagnetic structure. The magnetic susceptibility perpendicular to the c-axis of the crystal was measured as a function of temperature, and an abrupt increase in the susceptibility of 58% was observed in cooling through the transition. Above the transition the susceptibility is small, $2.38 \times 10^{-6} \text{emu/G}$, and virtually temperature-independent. This suggests that above the transition the compound exhibits Pauli paramagnetism, which is consistent with the metallic behavior observed. The comparatively small susceptibility below the transition is not fully understood as yet.

$\alpha\text{-Fe}_2\text{O}_3$ and FeS are two antiferromagnetic compounds known to possess spin rotation transitions in which the antiferromagnetic axis rotates approximately 90° at the transition temperature. The transition temperature for $\alpha\text{-Fe}_2\text{O}_3$ is sharp and occurs at 258°K , and for FeS⁵⁴ the rotation occurs over the interval $430\text{-}450^\circ\text{K}$. Previous neutron diffraction studies⁵⁰ of FeS indicated that there might be some change in the lattice parameters on passing through the transition. This point has been investigated⁵¹ carefully with improved accuracy in the location of the diffraction peak from which the lattice parameters are determined. In both $\alpha\text{-Fe}_2\text{O}_3$ and FeS distinct changes in slope of the lattice parameter vs temperature curves are observed at the spin rotation transitions. The linear expansion coefficients of $\alpha\text{-Fe}_2\text{O}_3$ above and below the transition are 9.78×10^{-6} and 4.65×10^{-6} , respectively. The linear expansion coefficients along the a-axis for FeS above and below the transition are 75.4×10^{-6} and 11.5×10^{-6} , respectively. The advantage of using neutron diffraction for this type of investigation is that both the magnetic properties and the lattice-parameter behavior can be investigated

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⁵⁰J. T. Sparks, W. Mead, and T. Komoto, J. Phys. Soc. Japan 17 B-1, 249 (1962).

⁵¹J. T. Sparks and T. Komoto, to be submitted to Acta Cryst. (1964).

simultaneously, allowing positive correlations to be made between changes in lattice parameters and changes in magnetic properties. This is not possible with x rays.

A paper has been written on a unique liquid-helium cryostat⁵² for neutron diffraction studies. This cryostat has been designed, constructed, and placed in operation. The cryostat allows investigations to be carried out at any temperature from liquid-helium temperatures to room temperature.

J. T. Sparks

M-Shell Fluorescence Yields of Bismuth, Lead, Gold, and Osmium

Very little is known about atomic fluorescence yields in the shells beyond the L shell. Only two previous references to measurements of M-shell fluorescence yields appear in the literature. One of these is an old (1934) measurement of an average M-shell fluorescence yield of uranium by Lay,⁵³ who used a photographic method to measure the intensity of the M x rays emitted by a uranium target following the ionization of the M shell by photoelectric absorption. The other is a more recent (1954) measurement of the M shell fluorescence yield of bismuth. This was done by measuring the intensity of the bismuth M x ray emitted by a RaD source and comparing this with the known decay rate of the source.⁵⁴ In view of this situation, it was decided to look again at the problem of measuring M-shell fluorescence yields to see whether techniques recently developed for L-shell measurements⁵⁵ could be profitably applied.

An important question which must be considered when attempting to measure M-shell fluorescence yields is the proper definition of the fluorescence yields. In the present experiments, M-shell vacancies are created by first producing L-shell vacancies which are subsequently filled by M-shell electrons. The M shell consists of five separate subshells. Electrons in each of these shells can make transitions to vacancies in one or more of the

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⁵²J. T. Sparks, T. Komoto and W. Wade, to be submitted to Rev. Sci. Instr. (1964).

⁵³H. Lay, Z. Physik 91, 533 (1935).

⁵⁴A. A. Jaffe, Bull. Res. Coun. Israel 3, No. 4, 316, (1954).

⁵⁵R. C. Jopson, Hans Mark, C. D. Swift, and M. A. Williamson, Phys. Rev. 136, A69 (1964).

three L subshells. Because of the complexity of the resulting spectrum and the poor energy resolution of the available detectors, great care must be exercised in defining the average M-shell fluorescence yield determined here in terms of the fluorescence yields of the individual M subshells.

The method employed in these experiments was similar to that used for previous measurements of L-shell fluorescence yields.⁵⁵ Thin foils of the materials to be studied were exposed to x rays or γ rays which could create vacancies in the L shells of the irradiated materials. The M-shell fluorescence yields were then determined by measuring the coincidence rate between the L and the M x rays observed following the L-shell ionization. It is shown that for the method used here the M-shell fluorescence yield determined is predominantly a combination of the fluorescence yields of the M_{IV} and the M_V subshells. The following values were obtained: bismuth, 0.037 ± 0.007 ; lead, 0.032 ± 0.006 ; gold, 0.030 ± 0.006 ; and osmium, 0.016 ± 0.003 .

R. C. Jopson, Hans Mark,
C. D. Swift and M. A. Williamson
(UCRL-7937)

Copper L_{III} Shell X-Ray Production by 25 to 100-keV Protons

Recent x-ray production studies of L-shell x rays from copper by proton bombardment (100-500 keV) have been extended to 25 keV energy.⁵⁶ In the region of the periodic table near copper the higher-intensity characteristic x-ray lines from the L_I and L_{II} shells are absorbed in the L_{III} shell. By using thin copper absorber foils, the characteristic x rays from the L_{III} shell of copper have been isolated from the L_I and L_{II} characteristic x rays. The thick-target yields of both groups were measured as well as the x-ray production cross section for the L_{III} shell (see Fig. 7). With a fluorescent yield of 0.05, the L_{III} shell ionization cross section decreases from $3.6 \times 10^{-22} \text{ cm}^2$ at 100 keV to $2.3 \times 10^{-24} \text{ cm}^2$ at 25 keV. The experimental cross sections are lower than theoretical predictions by over two orders of magnitude at 25 keV.⁵⁷ The $L_{III}/L_I + L_{II}$ x-ray intensity ratio decreases

⁵⁶J. M. Khan, D. L. Potter and R. D. Worley, Phys. Rev. 133, A316 (1964).

⁵⁷E. Merzbacher and H. W. Lewis, Encyclopedia of Physics (Springer-Verlag, Berlin, 1958) Vol. 34, p. 166.

Fig. 7. X-ray production cross section for the L_{III} shell in copper.

especially with hydrogen and helium isotopes. The yield for these light ions becomes particularly small as the energy of the ion approaches or exceeds 1 MeV.

Since a useful measurement of the yield from a given target should be made under clean surface conditions, the reduced yield associated with hydrogen or helium sputtering can cause a further complication. Ordinarily, the target surface is cleaned by the sputtering process itself which removes any impurities that may contaminate the surface. Since the target surface is cleaned at the rate at which surface particles are removed rather than at the rate at which ions arrive, surface contamination is more significant under the conditions of low-yield sputtering associated with 500-keV He^+ sputtering.

A radioactive tracer technique capable of measuring less than 10^{-10} g of copper has been developed. A 500-keV magnetically analyzed beam of helium ions is used to observe the sputtering yield as a function of carbonaceous film thickness over a copper target. It is shown that an amorphous film of the order of 2×10^{17} atoms/cm² reduces the sputtering yield of

from 1.4 at 100 keV to ~ 1 at 25 keV proton energy.

D. L. Potter, J. M. Khan,
and R. D. Worley
(UCRL-7813-T)

Effect of Thin Carbonaceous Films on 500-keV Helium Ion Sputtering of Copper

Measurement of the sputtering yield S (surface atoms ejected per bombardment ion) becomes increasingly difficult as the value of the yield decreases. Such measurements occur in seeking the threshold energy at which sputtering occurs,⁵⁸ and when sputtering with light ions; especially with hydrogen and helium isotopes.

⁵⁸R. V. Stuart and G. K. Wehner, J. Appl. Phys. 33, 7 (1962).

copper by a factor of 100. A first collision model of sputtered atom penetration of the film is in good agreement with the data and yields a copper-carbon cross section of $3 \times 10^{-17} \text{ cm}^2$. A clean-surface sputtering yield of 2×10^{-2} atoms/ion is obtained by extrapolation of the data and is consistent with the yield of 800 keV H_2^+ sputtering of copper reported by Kaminsky.⁵⁹ It is postulated that ordering of the amorphous film occurs for areal densities greater than $2 \times 10^{+17} \text{ atoms/cm}^2$ on the basis that the rate of reduction of copper yield with increasing film thickness undergoes a sharp decrease at that point.

H. P. Smith, Jr.,* D. W. DeMichele* and J. M. Khan
(UCRL-12022)

Energy Distribution of Gamma Rays in the Atmosphere

It was discovered a few years ago that a large flux of relatively soft gamma rays existed in the atmosphere.⁶⁰ These gamma rays are apparently in equilibrium with the primary cosmic ray beam striking the top of the atmosphere. The gamma rays observed in the low quantum energy region are probably either soft bremsstrahlung photons produced when shower electrons are scattered in the atmosphere, or they are the degraded photons resulting from successive Compton interactions by a higher-energy gamma ray. Measurements have already been performed in the energy range of 40 to 300 keV.⁶⁰ In this energy region, the photon flux observed at the highest energy is roughly one-fifth as large as that observed at the lowest quantum energies. The purpose of the present measurements was to extend the lower energy limit of the spectrum to about 5 keV and to learn something about the angular distribution of the photons. At the lower energies, the spectrum should eventually turn over and the observed photon flux should decrease as the quantum energy decreases. This must happen because at quantum energies below 50 keV, photoelectric absorption in the air is an important process. The expected turnover in the spectrum has been observed. It has also been demonstrated that the observed photon flux is roughly isotropic.

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*University of California, Berkeley, California.

⁵⁹M. Kaminsky, Phys. Rev. 126, 1267 (1962).

⁶⁰K. A. Anderson, Phys. Rev. 123, 1435 (1961).

Three series of balloon flights were made during the course of these experiments. The first was carried out on May 23, 1963 in Minneapolis, Minn. Two counters were mounted on one payload, one pointing up and the other pointing down. In July of the same year, several flights were made from Socorro, New Mexico. Smaller balloons were used so that only one counter could be mounted on a payload and still reach altitudes exceeding 100,000 feet. Four flights were made. However, due to bad weather, only one of these flights was successful. In July, 1964, two flights were made from the balloon launching site (NCAR) in Palestine, Texas. The first package was similar to the one flown in Minnesota and the second flight was used to determine various background effects.

The x-ray counter packages employed in all the flights were quite similar. A thin (~ 0.030 in.), cleaved NaI crystal was used as the x-ray detector. The crystals were mounted in an appropriate air-tight and light-tight holder. They were covered with thin beryllium windows (0.003 in.) to minimize absorption at low quantum energies. A conical collimator with an opening half angle of roughly 30° was mounted on top of the crystal holder. The crystal holder was optically coupled to the face of an RCA 6199 photomultiplier tube which was mounted on top of a compact power supply. The photomultiplier tubes employed in the package were especially selected for their low noise properties. With the photomultipliers operated at approximately 1000 V, it was possible to achieve a resolution of about 80% for the 6-keV iron K x-ray peak.

All of the flights conducted for these experiments had a very similar flight profile. The balloons were launched before noon and took roughly two hours to reach their maximum altitude, usually a little over 110,000 feet. They were then kept at altitude for two to five hours, depending on the conditions, after which the experiment was terminated.

The observed photon fluxes at 110,000 feet are shown in Fig. 8. Several conclusions can be drawn regarding the measurements described in this report:

- 1) At an altitude of 100,000 feet, the atmospheric gamma ray spectrum has a maximum between 30 keV and 50 keV. The photon flux at the maximum is roughly 2×10^{-2} photons-sec⁻¹-cm⁻²-keV⁻¹-sr⁻¹. The maximum seems to be at a slightly higher energy at 34° N than at 45° N.

Fig. 8. Photon spectrum at 110,000 feet (looking up).

2) At 50,000 feet, the altitude of the maximum ionizing radiation (Pfotzer maximum), the maximum of the gamma ray spectrum apparently occurs at slightly higher quantum energies — probably between 40 keV and 50 keV. The photon flux at this altitude at the maximum is about 4×10^{-2} photons-sec⁻¹-cm⁻²-keV⁻¹-sr⁻¹.

3) The observed gamma ray flux is roughly isotropic at both 100,000 feet and 50,000 feet.

4) There is a small latitude effect. The counting rates observed at Minneapolis (latitude 44° 58' N) are higher by approximately a factor of two than those observed in Texas (latitude 31° 46' N) and New Mexico (latitude 34° 05' N).

G. J. Chodil, R. C. Jopson,
Hans Mark and C. D. Swift

The Polarization of Neutrons from the $C^{13}(p, n_0)N^{13}$ and $N^{15}(p, n_0)O^{15}$ Reactions*

The angular distribution of the neutrons from the $C^{13}(p, n_0)N^{13}$ and $N^{15}(p, n_0)O^{15}$ reactions has been measured by Wong et al.⁶¹ for proton bombarding energies between 5 and 13 MeV. These studies were undertaken to investigate the suggestion of Bloom, Glendenning, and Moszkowski⁶² that one may be able to deduce the effective neutron-proton interaction inside the nucleus from measurements of the ground state (p, n) reaction on mirror nuclei. It was further suggested⁶⁴ that the above reactions are "twin" reactions; that is, the interaction could be considered as taking place between the incoming (outgoing) particle and a $p_{1/2}$ nucleon or nucleon hole in the field of a doubly closed shell nuclear core. The measurements of Wong et al. tended to corroborate this direct reaction concept in that the changes in the angular distributions as the proton bombarding energy is increased are quite gradual. The similarity of the two sets of angular distributions,

*A preliminary account of this work was presented at the American Physical Society 1964 Washington, D. C. Meeting: Bull. Am. Phys. Soc. 9, 444 (1964).

⁶¹C. Wong, J. D. Anderson, S. D. Bloom, J. W. McClure, and B. D. Walker, Phys. Rev. 123, 598 (1961).

⁶²S. D. Bloom, N. R. Glendenning, and S. A. Moszkowski, Phys. Rev. Letters 3, 98 (1959).

particularly at the higher energies, was also considered as confirming the twin reaction hypothesis.

In order to provide a more sensitive test of the twin reaction concept, the polarization of neutrons from the $C^{13}(p, n_0)N^{13}$ and $N^{15}(p, n_0)O^{15}$ reactions has been measured for proton energies in the region between 6.9 and 12.3 MeV and neutron emission angles between 0 and 90°. The neutrons were detected using the Livermore time-of-flight facility incorporating pulse-shape discrimination to reduce the time-independent background. The "left" and "right" measurements were obtained by using a solenoid for spin precession. Liquid helium was utilized as an analyzer. Large polarizations (50 to 70%) were measured for both reactions at several energies and angles. Corrections for multiple scattering in the analyzer have been made.

In addition, the measured polarizations were compared with quantitative polarization predictions obtained in the quasi-elastic interpretation of the (p, n) process. It has recently been pointed out by Lane⁶³ that the optical model potential should include a term proportional to $\underline{t} \cdot \underline{T}$ where $\underline{t}$ is the isospin of the incident nucleon and $\underline{T}$ is the isospin of the target nucleus. In addition to reproducing the proton potential anomaly,^{64, 65} this isospin term can induce a (p, n) reaction in which the target nucleus is converted into its corresponding isobaric state. Specifically this term can induce the (p, n₀) transitions of interest here since the ground states of N^{13} and O^{15} are the corresponding isobaric states of C^{13} and N^{15} . Quasi-elastic (p, n) reactions in nonmirror medium-A nuclei have been observed by Anderson et al.^{66, 67} and Batty et al.⁶⁸

Hansen and Stelts⁶⁹ have reported the angular distribution of the $N^{15}(p, n_0)O^{15}$ reaction along with the predictions obtained by treating the

⁶³A. M. Lane, Nucl. Phys. 35, 676 (1962).

⁶⁴A. E. Green and P. C. Sood, Phys. Rev. 111, 1147 (1958).

⁶⁵P. C. Sood, Nucl. Phys. 37, 627 (1962).

⁶⁶J. D. Anderson and C. Wong, Phys. Rev. Letters 7, 250 (1961).

⁶⁷J. D. Anderson, C. Wong, J. W. McClure, and B. D. Walker, Phys. Rev. (to be published).

⁶⁸C. J. Batty, G. H. Stafford and R. S. Gilmore, Phys. Letters 6, 292 (1963).

⁶⁹L. F. Hansen and M. L. Stelts, Phys. Rev. 132, 1123 (1963).

isospin potential as a perturbation in distorted wave Born approximation (DWBA).⁷⁰ These calculations which include the effects of the Coulomb field on the incident wave and the fact that the neutron energy differs from the proton energy by the Coulomb displacement energy in the distorting potentials gave fair agreement with experiment for proton bombarding energies between 5 and 12 MeV.

B. D. Walker, C. Wong, J. D. Anderson,
J. W. McClure, and R. W. Bauer*

UCRL-7676 (Rev. 1).

THERMODYNAMIC PROPERTIES OF MATTER

Theoretical

Quantum Corrections in the Thomas-Fermi Model

The simplicity of the Thomas-Fermi¹ model of the atom has made its appeal and use widespread, but has also led many to modify the theory in an effort to improve upon it and extend its range of validity. Of the various types of modifications which have been attempted we have been concerned with those intended to introduce quantum mechanical features not present in the simplest version of the theory. Such modifications, which can be introduced by any one of several procedures,²⁻⁶ all involve expansions in powers

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⁷⁰R. M. Drisko, R. H. Bassel and G. R. Satchler, Phys. Letters 2, 318 (1962).

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¹See P. Gombás, Die Statistische Theorie Des Atoms (Springer-Verlag, Vienna, 1949), for the standard references to the Thomas-Fermi model.

²W. R. Theis, Z. Physik 142, 503 (1955).

³A. S. Kompaneets and E. S. Pavlovskii, Soviet Physics JETP 31(4) 328 (1957).

⁴D. A. Kirznits, Soviet Physics JETP 32(5) 64 (1957). Unfortunately, the total energies calculated by Kirznits were omitted in the published translation. They are available in the original; Zh. Eksperim. i Teo. Fiz. 32, 115 (1957).

⁵S. Golden, Phys. Rev. 105, 604 (1957); Phys. Rev. 107, 1283 (1957).

⁶G. A. Baraff and S. Borowitz, Phys. Rev. 121, 1704 (1961).

of a small parameter which depends on Planck's constant and the atomic number, and lead to a supposedly improved model which includes exchange effects as well as terms related to the spatial dependence of the equivalent one-body potential provided by the theory.

Since these procedures for improving the Thomas-Fermi model depend upon expansions of certain physical quantities, the validity of the resulting corrections clearly depends crucially upon the validity of the expansions. Several recent investigations⁷⁻⁹ of this point show that, in special cases, expansions of the kind we are concerned with here yield asymptotic series valid only under certain conditions; further, it appears that the expansion procedure fails to yield terms of an oscillatory character which may be comparable in importance to the quantum corrections. These analyses have dealt only with one- and two-dimensional potentials linear and quadratic in the displacement, but an analysis of the expansion procedures in the case of the Coulomb potential in three dimensions which would have direct significance for atoms and ions has, to the best of our knowledge, never been made.

A numerical study of the quantum corrections to the Thomas-Fermi model of atoms and ions that are generated by any of the several equivalent expansion procedures has been made wherein corrected potentials, one-electron eigenvalues and eigenfunctions, dipole oscillator strengths, diamagnetic susceptibilities, and electron binding as a function of atomic number were considered. In all cases the corrected quantities either agree less well with experiment than the results of the simple zeroth-order theory or show improvement which is inconsistent, unimpressive, and unreliable, lending strong support to conjectures made by others that the expansion methods leading to the quantum corrections give rise to series which are asymptotic and which fail to include important oscillatory terms.

H. M. Schey and J. L. Schwartz
(UCRL-12042-T)

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⁷M. J. Stephen and K. Zalewski, Proc. Roy. Soc. (London) 435, A270 (1962).

⁸H. Payne, Phys. Rev. 132, 2544 (1963).

⁹N. Balazs, Phys. Rev. 134, A841 (1964).

Approximate Thomas-Fermi Potential

An approximate, finite-temperature Thomas-Fermi potential was arrived at from some physical considerations of a many-electron atom. The atom is divided into two regions; one of high and the other of low electron density. In the region of high electron density a potential closely resembling that used by Kerner¹⁰ for a zero temperature approximation to the Thomas-Fermi potential was used. In the region of low electron density the electron distribution was taken as uniform with a density approximately equal to the density at the surface of the atom. The slight deviation from equality was found by a first-order perturbation calculation.

The results of the approximate scheme were compared with those of Feynman, Metropolis, and Teller¹¹ and with Latter.¹² The agreement in potential was within a few percent for four cases compared in detail with Ref. 11. Electron pressures were within a few percent for all the cases calculated in Ref. 11.

The approximate scheme is quite easy to set up for machine calculation and runs rapidly. A case takes about two seconds on the IBM 7094 computer, and this could undoubtedly be reduced considerably by improving the convergence method. The accuracy of the scheme is probably well within the accuracy of the Thomas-Fermi model of the atom.

J. W. Zink
(UCRL-12054-T)

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¹⁰E. H. Kerner, Phys. Rev. 83, 71 (1951).

¹¹R. P. Feynman, N. Metropolis, and E. Teller, Phys. Rev., 75, 1561 (1949);

¹²R. Latter, Phys. Rev., 99, 1854 (1955), and RM 1227, A.E.C. (1954).

Phase Transitions of Repulsive Lattice Gas Models*

Following the discovery of the hard-sphere phase transition by Alder and Wainwright at Livermore,¹³ it has been suggested by several theoreticians that it may be possible to explain the solidification of gases under pressure by invoking only short-range repulsive forces between particles.¹⁴ Accordingly there has been considerable interest recently in the properties of various statistical-mechanical models of systems with repulsive forces, both from the viewpoint of making the models more realistic than the hard-sphere system, and for the purpose of gaining a better understanding of the mechanism of the transition.

The lattice gas is one type of model which can be used to study phase transitions of systems of particles with short-range forces. It is assumed that the particles may be located only at the nodes of a regular lattice of some type; no nodes may be occupied by more than one particle, and in general the number of particles is less than the number of nodes, so that the system may be regarded as a "mixture" of particles and "holes." Each particle interacts with its nearest neighbors, and possibly with second, third, etc. neighbors. The total potential energy of each arrangement of particles on the lattice is made up of contributions from neighboring pairs of particles, of the form

$$E = n_1 E_1 + n_2 E_2 + \dots,$$

where E_1 is the potential energy of a nearest-neighbor pair and n_1 is the number of such nearest-neighbor pairs, and similarly for E_2 , etc. Following

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*Based on a paper presented by R. Kikuchi at the American Physical Society meeting, Berkeley, December 1964. Abstract issued as UCRL-12116.

¹³B. J. Alder, and T. E. Wainwright, J. Chem. Phys. 27, 1208 (1957). The possibility of such a transition had previously been suggested by J. G. Kirkwood and E. Monroe, J. Chem. Phys. 10, 394 (1942), and by I. Z. Fisher, Zhur. Eksp. Teor. Fis. 28, 437 (1955) (Soviet Physics JETP 1, 273 (1955)). For reasons why there should not be a phase transition, see J. E. Mayer, Physics Today, January 1958, p. 22.

¹⁴See esp. H. N. V. Temperley, Proc. Phys. Soc. B70, 536 (1957); 74, 432 (1959); 77, 630 (1961) and later papers and preprints. Also: D. Turnbull and R. L. Cormia, J. Appl. Phys. 31, 674 (1960).

the usual methods of statistical mechanics, one writes down the partition function by enumerating all the possible arrangements, with the Boltzmann factor involving the energy of each arrangement. As soon as the partition function has been reduced to a simple form (usually by some kind of approximation) the thermodynamic properties of the system may be calculated. While it is possible in certain special cases to evaluate the partition function exactly and definitely determine what kind of phase transition (if any) is exhibited by the model, in most cases the problem of enumerating the arrangements cannot be solved precisely, and it has been found in the past that almost any type of approximation will have a qualitative effect on the nature of the phase transition. (For example, the Onsager solution of the two-dimensional Ising model shows a logarithmic singularity at the transition point, in contradiction to the approximate theories.) While one probably cannot hope, therefore, to obtain an exact description of the phase transition by approximate theories, previous experience shows that some types of approximations give fairly accurate results for the location of the singularity and for the values of thermodynamic properties for temperatures and pressures not too close to the transition temperature.

Probably the best approximate theory — judged by the criteria of accuracy as compared to known exact solutions and ease of application to more complicated models — is the "cluster-variation method" developed by Kikuchi and his co-workers.¹⁵ Like the earlier methods of Bethe¹⁶ and Guggenheim,¹⁷ it takes advantage of the fact that the thermodynamic properties of a system of a very large number of particles, while depending apparently on an average over all possible arrangements, actually depend essentially on only the most probable or equilibrium arrangement. The equilibrium arrangement will be characterized by a certain average number of nearest-neighbor particle-hole pairs, and by other similar parameters that are determined by the number of "clusters" of small groups of lattice nodes of various types. The number of arrangements corresponding to each possible set of values of these

¹⁵R. Kikuchi, Phys. Rev. 81, 988 (1951); M. Kurata, R. Kikuchi, and T. Watari, J. Chem. Phys. 21, 434 (1953), and later papers by Kikuchi.

¹⁶H. A. Bethe, Proc. Roy. Soc. London A150, 552 (1935).

¹⁷E. A. Guggenheim, Proc. Roy. Soc. London A169, 134 (1938); Mixtures (Oxford, 1952).

parameters is then approximated by assuming that the system can be divided into clusters which do not interfere with each other (i. e., have independent configurations). The Bethe-Guggenheim method makes use of one particular type of approximation at this step, while the Kikuchi method employs a somewhat different approximation which seems to be more accurate. Then one seeks the maximum term in partition function; in other words, one differentiates the product: (number of arrangements for set of values of parameters) $\times$ (Boltzmann factor for energy determined by that set) with respect to the values of the parameters, using Lagrange multipliers to ensure that certain auxiliary consistency conditions are satisfied. This process of determining the values of the parameters that give the largest term in the partition function is equivalent to searching for the macroscopic configuration of the system that has the lowest free energy, at least insofar as the parameters are directly related to observable properties of the system.

This approach is now being applied to lattice gas models in which each particle on a lattice node excludes other particles not only from its own node but also from a certain number N of neighboring shells of nodes. In the case $N = 0$ the model is equivalent to the well-known Ising model with repulsive interactions, which behaves somewhat like an antiferromagnet. Burley¹⁸ has studied the properties of this model using Kikuchi's method with squares and four lattice nodes as the basic cluster; we have extended this work by using cubes of eight nodes (simple cubic lattice). We find, in agreement with Burley's result, that there is an order-disorder transition corresponding to preferential occupation by the particles of one sub-lattice below a certain temperature, which depends on the density of particles. However, there is no first-order phase transition. Another similar model corresponds to $N = 2$: a particle at any node of a simple cubic lattice excludes other particles from the nearest-neighbor and next-nearest-neighbor positions, and there is a finite repulsive energy of interaction with particles at the third-nearest-neighbor position. In this case there is not only an order-disorder transition but also a first-order phase transition with a van der Waals loop. The pressure at the transition has a minimum with respect to increasing temperature.

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¹⁸D. M. Burley, Phil. Mag. 5, 909 (1960); Physica 27, 768 (1961); Proc. Phys. Soc. 75, 262 (1960), 77, 451 (1961).

At present it appears that the transition will become first-order for a certain critical value of N , possibly depending on the lattice type; this behavior is in agreement with Monte Carlo results of D. Chesnut for the triangular lattice (unpublished). It may have some relation to the hypothesis that for the "continuum" model in which the restriction to lattice positions is removed and the particles interact with repulsive forces inversely proportional to the n th power of the distance, the phase transition becomes first-order when n is greater than a certain critical value of n . (Unpublished results of W. Hoover at Livermore indicate that this critical n may be in the neighborhood of 150.)

S. G. Brush and R. Kikuchi

Pair Distribution Function of a Classical Electron Gas*

A Monte Carlo code known as TOWNLEY¹⁹ has been developed for generating and analyzing configurations of a few hundred particles interacting with inverse-power-law forces. The first application of the code has been to systems of 500 particles with repulsive Coulomb forces. One may imagine that there is a uniformly charged "background" in order to preserve charge neutrality, and to keep the system contained in a finite volume; however, in the systems studied so far the background actually plays no role and the system is contained simply by imposing periodic boundary conditions. Thus when a particle goes out one side of the box it comes back in on the other side. Each particle interacts with each of the other 499 particles in the box, or with the periodic "image" of a particle if the image is closer. The Monte Carlo technique is basically the same as that originally used for the hard-sphere system by Metropolis et al.²⁰ and by Alder et al.²⁰ we have adapted a

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*This report is based on a paper presented by S. G. Brush at the American Physical Society meeting, Plasma Physics Division, November 1964. An abstract was issued as UCRL-12099.

¹⁹In honor of the British scientist Richard Townley (1628-1707).

²⁰N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953); B. J. Alder, S. P. Frankel, and V. A. Lewinson, J. Chem. Phys. 23, 417 (1955).

code designed for an electrolyte system by J. Shaw.²¹ The particles may be started from a specified set of positions, or may be located at random. The random numbers are generated by the RNFL subroutine available at Livermore, which is based on the method proposed by Lehmer.²² By moving one particle at a time, one constructs a Markov chain of configurations which can be shown to have the properties of a canonical ensemble if the chain is long enough and the transition probabilities are chosen properly.²⁰

For the system of particles with charge Ze each, the physical state of the system is characterized by a single dimensionless parameter s :

$$s = (Ze)^2/kTa,$$

where a = ion sphere radius = $(3/4\pi n)^{1/3}$ and n = number density. Runs of about 100,000 configurations each were obtained for $s = 0.2, 1, 2, 5$, and 10 . For $s = 0.2$, results in agreement with the Debye-Hückel formula

$$g_{DH} = \exp \left\{ -\frac{s}{r} e^{-r\sqrt{3s}} \right\}.$$

For $s = 1$, significant deviations from the Debye-Hückel result are observed, and the results are closer to those calculated from the Percus-Yevick equation by Carley.²³ Our results for this value of s are also in close agreement with unpublished "molecular dynamics" calculations by W. Hoover of Livermore for a 64-particle system. For larger values of s , the value of the pair distribution function falls considerably below the Debye-Hückel value at small interparticle distances and rises above it at distances corresponding to the first nearest neighbor position. At $s = 10$, the distribution function has a distinctly oscillatory character indicating the presence of short range order.

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²¹J. N. Shaw, Monte Carlo Calculations for a System of Hard-Sphere Ions, Ph. D. Dissertation, Duke University, 1963.

²²See L. J. Gannon and L. A. Schmittroth, AEC report IDO-16921 (Aug. 20, 1963) for discussion of this method of generating random numbers, and references cited therein.

²³D. D. Carley, Phys. Rev. 131, 1406 (1963).

We are now making shorter runs at higher values of s in order to determine the location of the transition to a lattice structure, and to establish what type of lattice is most stable.

S. G. Brush, H. L. Sahlin and E. Teller

Calculation of Virial Coefficients for Squares and Cubes with Attractive Forces

The equation of state relates the pressure P , volume V , temperature T , and number of particles N to each other. For gases this relation is conveniently written in the so-called virial form:

$$PV/NkT = 1 + B_2(T)\rho + B_3(T)\rho^2 + B_4(T)\rho^3 + \dots; \rho = N/V.$$

The coefficient of ρ^{n-1} in this expansion is called the n th virial coefficient. From Mayer's work²⁴ each of the virial coefficients can be calculated (in principle) from the interparticle force law. Each virial coefficient B_n can be expressed as a sum of integrals of functions of the forces exerted by n interacting particles. In general, these integrals are difficult to evaluate and virial coefficients beyond the third are rarely calculated. For interparticle forces which are completely repulsive it is possible to go somewhat farther than B_3 . For hard-sphere particles the coefficients B_5 and B_6 were recently calculated (within 1%) by a Monte Carlo method.²⁵ For hard-cube particles the first seven virial coefficients have been calculated exactly.²⁶ For particles with attractive as well as repulsive forces the situation is not so pleasant. For the simplest such model, hard spheres with a "square-well" attraction, the first three virial coefficients have been evaluated exactly, and the fourth approximately.²⁷

We have discovered that for particles which interact with cubic rather than spherical attractive wells it is possible to work out the first five virial coefficients analytically. The simplification which makes this possible is

²⁴J. E. Mayer and M. G. Mayer, Statistical Mechanics (John Wiley & Sons, Inc., New York, 1940). Chapter 13 describes the theoretical determination of virial coefficients.

²⁵F. H. Ree and W. G. Hoover, J. Chem. Phys. 40, 939 (1964).

²⁶W. G. Hoover and A. G. DeRocco, J. Chem. Phys. 36, 3141 (1962).

²⁷See J. A. Barker and J. J. Monaghan, J. Chem. Phys. 36, 2558 (1962).

the reformulation of the force integral problem in terms of a combinatorial problem which can be solved by a high-speed computer. We have obtained the first five virial coefficients for both two- and three-dimensional gases with square-well attractions.²⁸

Once one has these virial equations of state there are several questions worth asking about the results. The first might well be how useful is the truncated virial series near the gas-liquid critical point? We were able to check on this point by computing the critical points (inflection points in a plot of pressure vs density) for the three-, four-, and five-term virial series. We found that the individual critical parameters were very sensitive to the number of terms retained in the series so that P_c , V_c , and T_c cannot be reliably estimated from truncated series. The product $P_c V_c$ is remarkably constant, however. In three dimensions the reduced (dimensionless) values of $P_c V_c$ at the critical point were 1.05, 1.01, and 1.10 for the three-, four-, and five-term series, respectively. This indicates that virial coefficient calculations can lead to rather reliable estimates of the pressure-volume product at the critical point.

We were also able to prove, for the particles we considered, that all of the virial coefficients beyond the second become negative as the temperature approaches zero. This property has been assumed by most people since Mayer's early work, but ours is the first proof of this property for a reasonably realistic force function.

Finally, we were able to show that physical clusters of n particles make the dominant low-temperature contribution to the n th virial coefficient B_n . It had previously been stated²⁹ that the low-temperature virial coefficients were determined in form by the so-called "complete star" integral, but we have shown that this is false. We find that $\ln|B_n|$ approaches n/T at low temperature, while the complete star contribution, which is of order n^2/T , is completely offset by other integrals contributing to B_n .

This work is described in detail in Ref. 28, which has been submitted to the Journal of Chemical Physics for publication.

W. G. Hoover and F. H. Ree

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²⁸W. G. Hoover and F. H. Ree, "Calculation of Virial Coefficients. Squares and Cubes with Attractive Forces." UCRL 7950-T.

²⁹S. Katsura, Phys. Rev. 115, 1417 (1959).

Hard-Sphere Bulk Viscosity

The bulk viscosity of a system of a system of hard-sphere molecules has been calculated from the autocorrelation of the diagonal terms in the stress tensor using the technique previously employed to calculate the shear viscosity.³⁰ As in the previous case, the autocorrelation function is separated into a kinetic part, a potential part, and a mixed part involving both velocities and forces. The kinetic part and the mixed part are assumed to be exponentially decaying functions of time which are determined by the initial value and the initial rate of decay. These two parts give rise to the first two terms (D_1 and D_2) in the viscosity, which is written in the following form:

$$\frac{\kappa}{\eta_0} + \frac{4}{3} \frac{\eta}{\eta_0} = \frac{B}{yV} (D_1 + y D_2 + y^2 D_3)$$

where κ and η are the bulk and shear viscosities, B is the second virial coefficient, and V is the volume per molecule. $y \equiv PV/kT - 1$. D_1 and D_2 are found to be $4/3$ and $16/15$, respectively, in agreement with the Enskog³¹ theory.

The term D_3 , which arises from the potential part of the autocorrelation, is calculated by means of sum of an infinite series of terms rather than the integral of an exponentially decaying function as in the case of D_1 and D_2 . As in the case of the shear viscosity calculation, only the first two terms of the series are actually calculated. In the present case the series does not seem to converge as rapidly as it did in the shear viscosity calculation so that the sum inferred from the first two terms is not so reliable. The result of D_3 is 2.19, which is in only fair agreement with the Enskog theory which would require a D_3 of about 2.02.

T. E. Wainwright

³⁰J. Chem. Phys. 40, 2932 (1964).

³¹See S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases (Cambridge University Press, 1939).

Numerical Solution of the Schrödinger Equation with the Complete Screened Coulomb Potential*

The complete screened Coulomb potential for a Debye-Hückel ion atmosphere is given by³²⁻³⁴

$$V(r) = \begin{cases} V_i(r) = -Ze^2 \left(\frac{1}{r} - \frac{1}{D+a} \right), & r \leq a \\ V_0(r) = -Ze^2 \frac{D}{D+a} \frac{\exp[(r-a)/D]}{r}, & r \geq a \end{cases} \quad (1)$$

where D is the Debye length and a is the minimum radius of the ion atmosphere.^{34, 35} With the transformation $\rho = (2A/a_0 n)r$ (a_0 = radius of the first Bohr orbit), the radial Schrödinger equation for a hydrogenic ion becomes

$$\frac{1}{\rho} \frac{d}{d\rho} \left(\rho^2 \frac{dR(\rho)}{d\rho} \right) + \left\{ -\frac{1}{4} - \frac{\ell(\ell+1)}{\rho^2} + nv(\rho) \right\} R(\rho) = 0 \quad (2)$$

where $v(\rho)$ is the transform of $V(r)$ in (1) divided by Ze^2 (see Ref. 36). As with the standard Coulomb potential, the eigenvalues of Eq. (2) are given by

$$W_n = -\frac{\mu e^4}{2\hbar^2 n^2} \quad (3)$$

Preliminary ground-state solutions of Eq. (2) have been obtained with $\ell = 0$ for variations of n as a function of a and D . Curves of D vs n are plotted in Fig. 9 for the two cases $a = D$ and $a = 0$.

Clearly, the standard Coulomb solution with $n = 1.0$ is the limiting case of a and/or $D \rightarrow \infty$, and represents an ideal, isolated atom. Solutions

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*Bull. Am. Phys. Soc. Ser II 9 No. 7 (1964).

³²H. Margeneau and M. Lewis, Rev. Mod. Phys. 31, 569 (1959).

³³T. L. Hill, An Introduction to Statistical Thermodynamics (Addison-Wesley Publishing Co., Inc. 1960).

³⁴C. A. Rouse, "A Note on the Maximum Bound Principal Quantum Number," 6th Int. Conf. on the Phys. of Ionized Gases, Paris, 1963.

³⁵E. Meeron, "Statistical Mechanics of Reversible Processes in Plasma Dynamics," in Plasma Physics, Ed. J. E. Drummond (McGraw-Hill Book Co. Inc., New York, 1961).

³⁶C. W. Sherwin, Introduction to Quantum Mechanics (Holt, Rinehart and Winston, New York).

Fig. 9. D vs n for potentials with where
(1) $a = D$ and (2) $a = 0$. Solutions represent ground states of hydrogenic ion ($\ell = 0$).

$$C_{p_1 p_2 k_1 k_2} = e^2 \int \int \phi_{p_1}^*(r_1) \phi_{p_2}^*(r_2) \frac{1}{r_{12}} \phi_{k_1}(r_1) \phi_{k_1}(r_2) dr_1 dr_2.$$

The $\phi(r)$ are hydrogen-like wave functions

of Eq. (2) with Eq. (1) represents first-order effects on the ground-state of a nonisolated hydrogenic ion by an ion atmosphere.

C. A. Rouse

Calculation of Helium Energies

Schrödinger's equation for the electrostatic helium atom

$$\left(-\frac{\hbar^2}{2m} \nabla_{r_1}^2 - \frac{\hbar^2}{2m} \nabla_{r_2}^2 - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}} \right) \psi = E' \psi$$

can be transformed to the infinite degree secular equation^{37, 38}

$$\sum_{k_1=1}^{\infty} \sum_{k_2=1}^{\infty} \left[C_{p_1 p_2 k_1 k_2} + \left(E_{k_1 k_2} - E'_{p_1 p_2} \right) \delta_{p_1 k_1} \delta_{p_2 k_2} \right] M_{p_1 p_2 k_1 k_2} = 0,$$

³⁷ J. C. Slater, Quantum Theory of Atomic Structure (McGraw-Hill Book Co., Inc., New York, 1960) Volume I, Chapter 5.

³⁸ J. E. Swain, "Helium Isoelectronic Sequence Wave Functions and Energies of the Second and Third Rows of the Periodic Table," UCRL 7842-T.

$$\left(-\frac{\hbar^2}{2m} \nabla_r^2 - \frac{Ze^2}{r} \right) \phi_k = E_k \phi_k.$$

The helium wave function ψ has been expressed as

$$\psi_{p_1 p_2} = \sum_{k_1=1}^{\infty} \sum_{k_2=1}^{\infty} M_{p_1 p_2 k_1 k_2} \phi_{k_1}(r_1) \phi_{k_2}(r_2).$$

The energy $E_{k_1 k_2}$ is

$$E_{k_1 k_2} = E_{k_1} + E_{k_2}.$$

Approximations to the solution of Schrödinger's equation are made by truncating the infinite-degree secular equation. Two truncated secular equations, one 25×25 and the other 196×196 , have been solved. Energies and wave functions are obtained for the 1^1S , 2^1S , 2^3S , 2^1P , and 2^3P states from the 25×25 approximation, and the 1^1S , 2^1S , 2^3S , 2^1P , 2^3P , 3^1S , 3^3S , 3^1P , 3^3P , 3^1D , and 3^3D states from the 196×196 approximation.³⁹

Table 1 compares the energies obtained from the (25×25) and (196×196) calculations with experimental values.

From this table it is noted that the convergence is poor for the 1^1S state, very good for the 2^3S , 2^1S , 2^3P , and 2^1P states and as yet undetermined for the remainder of the states.

With small effort accurate energies can be calculated using the secular equation approach.

J. E. Swain

³⁹J. E. Swain and B. Curnutte, Jr. "Comparison of the First Three Approximations to the Wave Functions and Energies of the Helium Isoelectronic Sequence," UCRL 7941-T.

Table 1. Helium energies.

State	25 X 25	196 X 196	Experimental
(1S ²)1 ¹ S	-77.15282 eV	-77.41097 eV	-78.983 eV ^a
(1S, 2S)2 ³ S	-57.83002	-59.07635	-59.170
(1S, 2S)2 ¹ S	-53.32694	-58.16454	-58.374
(1S, 2P)2 ³ P	-55.81225	-58.00456	-58.025
(1S, 2P)2 ¹ P	-52.04602	-57.73372	-57.772
(1S, 3S)3 ³ S	-	-54.45086	-56.272
(1S, 3S)3 ¹ S	-	-49.74764	-56.070
(1S, 3P)3 ³ P	-	-52.65249	-55.983
(1S, 3P)3 ¹ P	-	-50.52697	-55.903
(1S, 3d)3 ³ D	-	-54.46717	-55.916
(1S, 3d)3 ¹ D	-	-54.45086	-55.916
(2S ²)1 ¹ S	-20.47162	-20.968071	-

^aG. E. Moore, Atomic Energy Levels, (N. B. S. Circular 467, Washington, D. C., 1949) Volume I.

Experimental

Properties of Materials

Properties of compressed magnetic oxides. Measurements of the demagnetization of nickel ferrite (NiFe₂O₄) under shock compression and heating have been made. In these experiments, samples are biased to saturation by a permanent magnet. The shock-induced reduction in magnetic flux through the sample is detected by pickup coils, which are wound on the ferrite cores completing the magnetic circuit between the sample and the biasing magnet. The flux change is determined by integrating signals from the coils. Within an experimental uncertainty of $\pm 10\%$, this flux change was identical in five shots at pressures between 140 and 430 kbar. This independence of the effect on shock pressure indicates that complete demagnetization had taken place. Temperature calculations based on equation of state measurements on the shocked material indicate that the Néel temperature decreases by 3 deg/kbar from the value of 590°C in the uncompressed material. At the lowest pressure, the effect took place as a two-step process. Half of the demagnetization occurred on the passage of an apparently elastic wave, and

the remainder on the passage of the plastic wave. The effect of incomplete initial saturation was measured, and the validity of corrections for this effect was confirmed. Approximate corrections for edge effects and for the position of the pickup coils were also made on the observed flux change. This corrected flux agrees with the saturation magnetization measured in a static experiment to within the experimental uncertainty. There is some evidence of a possible rate effect in the demagnetization. Future work will attempt to increase the accuracy of the measurements by checking the validity of certain geometrical corrections and will extend this work to lower pressures.

E. B. Royce

Shock-Induced phase transitions using a quartz gage. A quartz pressure gage technique⁴⁰ has been used successfully to observe multiple wave structures associated with phase transitions in bismuth, potassium chloride, and potassium bromide.

Dynamic transition pressures between 23.5 and 28.5 kbars have been observed in bismuth. It is felt that this transition is the same one observed statically at 25 kbars and room temperature. The scatter in the dynamic data appears to be due to temperature, sample thickness, and driving pressure effects. The temperature effect is easily adjusted, but the contributions from the other effects are unknown. More assemblies are now being fabricated to test the effects of sample thickness and driving pressure.

In order to have a better understanding of the bismuth transition, single crystals are now being grown. The low pressure phase of bismuth is rhombohedral and is converted to a second phase of unknown crystal line structure. It appears possible that a single crystal shocked perpendicular to the trigonal axis might not undergo such a phase transition. If this were true, the hydrostatic assumption for dynamic systems above yield would not be valid. These experiments should clarify this point. The single crystals should also give a clear-cut dynamic yield point so that strength-of-material effects can be included in the comparison of the dynamic and static transition pressures.

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⁴⁰R. A. Graham et al., "Piezoelectric Current from Shock Loaded Quartz-A Submicrosecond Stress Gage," submitted to the Journal of Applied Physics, 1964.

Transitions at 16.7 kbars in KCl and 16.4 kbars in KBr have been observed. Statically KCl has a transition at 19.3 kbars and KBr has one at 17.9 kbars. These transitions are from face-center cubic to body-center cubic. Dynamic experiments at different thicknesses and temperatures on two different orientations of single crystals will be carried out in the near future.

The KCl, KBr alkali halide systems are comparatively simple from a theoretical point of view, and perhaps these experimental data obtained with the quartz gage can be useful to a theoretical investigation.

A clear understanding of these three transitions may lead to the use of other shock-wave phase transition points as calibration points for the highest ranges of pressure.

D. B. Larson

Equation of State Measurements

Equation of state compendium I. Data obtained with shock wave techniques are being compiled in tabular form in a compendium of equation of state data. The compilation is designed as a loose-leaf volume with a page for each data source. The filing numbers are based on the finding number system of the periodic table used by the Bureau of Standards for their "Consolidated Index of Selected Property Values."⁴¹ This allows a flexible system to which pages can be added or changed at will.

A computer program is being written to put the compilation on tape. The following retrieval capabilities are felt to be desirable and will be incorporated in the system program:

- (1) Printing of all data on the tape in order of the filing number. This may not be the order on the tape because of successive additions.
- (2) Printing of certain selected materials.
- (3) Generation of a source index.
- (4) Generation of a materials index.
- (5) Generation of graphs of selected data columns.

Laboratories in and outside of the United States engaged in shock wave work who may be potential contributors have been contacted.

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⁴¹Consolidated Index of Selected Property Values, Publication No. 976, National Academy of Science, 1962.

Interpretation of experiments done at pressures near the elastic yield point are still in a state of flux. Efforts are being made to find an adequate characterization of samples in this range as well as a reasonable standard method of presenting the data.

M. Van Thiel and V. W. Davis

The dynamic equation of state of rocks. Most of the Ester data of the Hugoniot equation of state of rocks was recently reanalyzed and supplemented for most rocks with sound velocity measurements and mineralogical and chemical analysis.

A similar summary was published by D. Lombard in 1961.⁴²

The samples in an Ester experiment^{43, 44} are placed on a plate with a known Hugoniot, the shock free surface velocities are recorded by optical flash technique, and the particle velocities and pressure are obtained from the solution of the dynamic impedance matching conditions.

Only the data for high pressure are included in the summary of results, since the Ester experiment cannot resolve the multiple shock fronts which occur at lower pressures. The data are shown in Figs. 10 and 11.

A detailed discussion of the Ester experiment can be found in R. Christian's thesis,⁴³ and similar techniques are discussed by Rice, McQueen, and Walsh.⁴⁴

The following rocks were investigated:

Andesite, Marin County	$\rho_{av} = 2.624$
Basalt, Nevada Test Site	$\rho_{av} = 2.675$
Granite (pink and grey), Nevada Test Site	$\rho_{av} = 2.676$
Idaho Black Rock, Bruneau Canyon, Idaho	$\rho_{av} = 2.464$
Limestone (Solenhofen)	$\rho_{av} = 2.584$
Limestone (Pony Creek), Alberta, Canada	$\rho_{av} = 2.577$
Oil Sand, Alberta, Canada	$\rho_{av} = 1.895$
Taconite "iron," Masabi Range, Erie Formation	$\rho_{av} = 4.325$
Tuff (red), Nevada Test Site	$\rho_{av} = 1.905$

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⁴²D. B. Lombard UCRL 6311 (1961).

⁴³R. H. Christian UCRL 4900 (1957).

⁴⁴Solid State Phys. 6, 59 (1958).

Fig. 10. Pressure as a function of particle velocity for selected rocks: a summary of Ester data.

Fig. 11. Shock velocity as a function of particle velocity for selected rocks: a summary of Ester data.

Tuff (white), Nevada Test Site

$\rho_{av} = 1.663$

Tuff (wet), Nevada Test Site

$\rho_{av} = 1.889$

A. Kusubov

Experimental Methods, Techniques, and Instrumentation

Absorption spectroscopy of compressed samples II. The development of absorption spectrometric methods to study the spectrum of shocked samples is continuing. It was found desirable to increase the duration of the flash light source. This allows a direct calibration of the source intensity. A source with useful flash duration of about 10 μ sec has been made and tested. It consists of a 3/4-in. -long by 1/2-in. -o.d. tube made of 9404 explosive with a 1/8-in. axial hole. The tube was detonated at one end by an SE-1 detonator and a 1/2-in. tetryl pellet. The detonation compresses a stream of argon gas introduced through a small hole in the tube wall just under the tetryl pellet. Explosive and detonator are surrounded by a metal tube.

The light from this source was passed into a shocked sodium-chloride pellet at a 60° angle to the shock front. It was reflected back out of the sample by a polished dural base plate through which the shock was passed. The spectrum of the reflected light beam was obtained as mentioned in a previous report. Some reduction of the reflected light was apparent. This is probably due to the change in reflectivity of the base plate in the visible range (7000 - 3500°) of the spectrum under a shock pressure of 130 kbars. The spectral analysis is still in progress.

A. C. Mitchell and M. Van Thiel

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Inclined mirror equation of state measurements. Equation of state measurements in the low pressure region ($P < 200$ kbar) are complicated by the presence of multiple wave structures arising from phase transitions or from elastic-plastic effects. Continuous measurements of free-surface velocity or position afford one method of resolving such structures. Such measurements have been made using a mirror inclined at a small angle to the free surface of an equation of state sample. The reflectivity of each region of the mirror changes as the free surface comes into contact with that particular region of the mirror. The mirror is illuminated by an argon

candle and viewed with the usual streaking camera, focused on the mirror. The technique has been successfully tested by measuring the equation of state of aluminum and will be used for measurements on ceramic materials. It is similar to a technique developed at the Stanford Research Institute.

W. H. Gust and E. B. Royce

FLUID AND HYDRODYNAMICS

Theoretical

Similarity Solutions in 1-D Hydrodynamics

The study of the hydrodynamics of compressible fluids and its applications to physical systems is facilitated in many ways by the availability of particularly simple solutions. The major class of these solutions for one-dimensional problems (in plane, cylindrical or spherical symmetry) are the "similarity," or "progressive wave" solutions. Of these the largest and most useful class exist for fluids with a γ -law equation of state, although in general some kinds of similarity flow exist for the most general equation of state. For a γ -law fluid the theory of similarity solutions reduces to its simplest form and is applicable, as we shall see, to the widest range of boundary value or initial value problems.

Similarity solutions appear typically as the asymptotic solution of a hydrodynamic problem. Even though in many applications the asymptotic solution is not physically interesting, it is nevertheless important and convenient in computations to know how it should behave.

An extensive and systematic treatment of the application of similarity theory to hydrodynamics by analogy with methods of dimensional analyses is given in Sedov.¹ Courant and Friedrichs² give a less complete discussion under the name of "progressing waves." Sedov's treatment is followed more closely here.

Two new examples of similarity solutions have been performed. In the first example the familiar Taylor blast wave, a similarity solution representing the asymptotic form of a blast wave in an atmosphere with a γ -law equation

¹Sedov, L. I., Similarity and Dimensional Methods in Mechanics, Chapter IV (Academic Press, New York, 1958).

²Courant, R. and Friedrichs, K. O., Supersonic Flow and Shock Waves, Chapter VI C (Interscience Publishers, Inc., New York (1948).

of state, has been generalized to apply to an atmosphere with a more realistic equation of state. In a second application, the initial pile-up of fluid material in a simple rarefaction wave against a rigid wall has been shown to be described by a similarity solution. Numerical calculations for both examples have been performed by an IBM 7094 computer code SIMS³ which calculates γ -law similarity solutions.

R. Grover
(UCRL-12018-T)

Numerical Treatment of Turbulent Flows^{*}

The grid size establishes a lower limit to the scales of motion resolved explicitly in finite difference models of turbulent hydrodynamic flows. Though the initial state of a flow may involve only larger scales of motion, nonlinearity leads to motions of smaller scale. This cascading of energy from larger to smaller scales can carry energy out of the resolved scales in a way improperly described by a finite difference scheme.

To provide energy removal, Smagorinsky⁴ introduced a viscosity ν depending on the grid scale λ and on the energy cascade rate ϵ . If ν depends only on λ and ϵ , dimensional considerations require $\nu = \alpha \epsilon^{1/3} \lambda^{4/3}$, where α is dimensionless. This ν can be considered an eddy viscosity diffusing large-scale momentum by small-scale turbulence. The large-scale energy dissipation ϵ is in turn dependent on the large-scale deformation rate D . From $\epsilon = \nu D^2$ one finds $\nu = \alpha^{3/2} D \lambda^2$.

For one-dimension, $D = |\Delta u / \Delta x|$, $\lambda = \Delta x$, $\nu = \alpha^{3/2} |\Delta u| \Delta x$ and the viscous stress $q = -\nu (\Delta u / \Delta x) = -\alpha^{3/2} |\Delta u| \Delta u$ has the form of a nonlinear artificial viscosity proposed by von Neumann and Richtmyer.⁵

C. E. Leith
(UCRL-12114-T)
(Abstract)

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^{*}(Invited paper to be presented at meeting of American Institute of Aeronautics and Astronautics - New York, January, 1965.)

³R. Grover UCRL-12018-T.

⁴J. Smagorinsky, Mon. Wea. Rev. 91, 319 (1963).

⁵J. von Neumann and R. Richtmyer, J. Appl. Phys. 21, 232 (1950).

Lagrange Representation with Time-Independent Mass Density

Much of the current work in hydrodynamics is empirical. Problems are formulated in particular representations, approximations made, computational techniques devised, and limitations of all these frequently encountered.

The investigation reported below is intended to furnish a general framework into which these various endeavors could be fitted, and hopefully, to suggest a method for getting around some of the difficulties they encounter.

The differential manifold $(\underline{x}, t)$ of conventional hydrodynamics with the transformations

$$M^{(3)} : \begin{array}{l} \underline{x} \rightarrow \underline{x}' = f(\underline{x}) \\ t \rightarrow t' = t \end{array}$$

is generalized to $(\underline{x}, t)$ with

$$M^{(3-1/2)} : \begin{array}{l} \underline{x} \rightarrow \underline{x}' = f(\underline{x}t) \\ t \rightarrow t' = t \end{array}$$

The invariant exterior differential calculus of $M^{(3)}$ (divergencies, curls, Stokes' and Green's theorems) is preserved under this extension. Into $M^{(1/2)}$ we introduce something new: a kinematic connection, a concept modeled after the affine connection of Ricci. The latter is based on a metric, the former is based on a velocity field. This new structure permits the definition of an invariant time derivative, compatible with the operations of the exterior calculus.

In this invariant language we now formulate the hydrodynamic laws of balance and inertia and the laws of thermodynamics. It is through the law of inertia that the time-dependent metric of space assumed dynamical significance, and we obtain an equation of motion for it.

We now single out two frames: the Lagrange, in which the velocity of the kinematic connection vanishes, and the Euler, in which it turns out to be the contravariant component of the covariant momentum vector. The latter identification is the hydrodynamic analogue of the "ether relations"

$(\underline{D} = \underline{E}; \underline{H} = \underline{B})$ of electromagnetic theory.

This scheme permits a Lagrange representation with time-independent mass density for any number of dimensions. In it, a holonomic transition between the Euler and Lagrange representations is contingent upon the integrability of a set of partial differential equations for the metric.

An investigation of the possibility that the structure of the class of transformation from the Euler to the Lagrange frames may point to a non-statistical theory of turbulence has been carried out.

At the outset of the investigation it was necessary to give up the generally accepted notion that the Euler and Lagrange representations are two equally valid descriptions of the dynamic system. The Lagrange form with its momentum and without kinetic velocity is now taken as the fundamental dynamic manifold. Because of the curvature associated with its geometry it cannot in general be charted on a single Euclidean space, customarily associated with the Euler representation. Rather a whole atlas of such charts may be necessary. Each of these Eulerian charts would then correspond to a small, smooth piece of fluid in turbulent motion.

The transformations from the Euler to the Lagrange picture contain in them the kinetic velocity as a parameter. This velocity suffers discontinuities when moving from one neighborhood to another. It is hoped that a closer investigation of these will yield a more quantitative description of turbulence.

Maurice Neuman

Applied

Numerical Simulation of the Earth's Atmosphere

The development of high-speed computers has permitted in the last 15 years a new approach to one of man's oldest scientific problems: the understanding and prediction of the behavior of the earth's atmosphere. By the beginning of this century the problem was recognized as a purely computational one. The fundamental laws of hydrodynamics and thermodynamics which the atmosphere obeyed were well known; it was thought only necessary to integrate the appropriate differential equations to find the state of the atmosphere for all future time. The attempt of L. F. Richardson⁶ started in 1911 to do just this by hand calculation showed the magnitude of the task. In fact, the problem is of such a magnitude that the fastest present-day computers are needed for calculations of the larger cyclonic scales of motion, leaving for the future numerical models sufficiently refined to include the detail of frontal systems. There is, however, much to be learned

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⁶L. F. Richardson, Weather Prediction by Numerical Process (Cambridge University Press, London, 1922) pp. 236.

at the present level of definition about the mechanisms by which heat and momentum are transferred from one latitude to another, about predictability of atmospheric motions, and about the dependence of the average state of the atmosphere on such things as albedo and temperature of the earth's surface.

One such numerical model of the atmosphere has been developed over the last few years. In this model an attempt is made to compute the hydrodynamic and thermodynamic evolution of a moist atmosphere on the whole globe taking into account such external influences as solar heating, evaporation, and surface friction. The equations used for this are those describing the thermodynamic relations and conservation of mass, momentum, energy, and water vapor.

The numerical model approximates by finite difference equations the hydrodynamic and thermodynamic laws appropriate to a three-dimensional moist atmosphere. The grid used divides the atmosphere into six pressure levels in the vertical and covers the globe with a horizontal grid spacing of about 300 miles. The numerical problems of finding a stable and reasonably accurate advection difference approximation, as well as the problem of taking into account turbulent and convective motions of a scale smaller than grid size, have been investigated.

Heating is computed as due to incoming solar radiation and to the release of latent heat that occurs when water vapor condenses. Evaporation serves as a source of water vapor which condenses and produces precipitation when saturation conditions are reached. Also included are the effects of frictional interaction and small-scale convective heat flux at the earth's surface.

All these influences are involved in a computational cycle that advances the state of the atmosphere by 10 minutes, and which can be iterated for months of atmosphere time.

C. E. Leith
(UCRL-7986-T)

Model Atmosphere

An improvement in the treatment of the surface-layer physics has led to more realistic differences between water and air temperatures at the surface and thereby solved a former problem of runaway convective rainfall cells in the tropics.

A rather fundamental change in the finite difference equations has been introduced that has removed several minor instabilities that arose from the interaction of the difference schemes (stable by themselves) used for different parts of the physics. The new technique involves applying the different schemes in sequence rather than in parallel, maintaining thereby the stability of the individual factors. The present form of the numerical model is described in a recent report.⁷

An experiment is being carried out to test the predictability of the model and to shed some light on the predictability of the atmosphere. At an arbitrary time in a calculation the temperature field in the atmosphere has a perturbation of simple form and 1° C amplitude applied. The resulting perturbed behavior is being compared with the unperturbed behavior to discover how rapidly slightly different states of the atmosphere diverge. This is being done in part to answer questions about the economic worth of various proposed extensions of the observation network. The preliminary results of this experiment indicate a degree of predictability higher than expected.

C. E. Leith

Evaluation of Spectral Versus Grid Methods of Hemispheric Numerical Weather Prediction

Using observed hemispheric meteorological data as initial conditions, typical barotropic (one-level) filtered-equation numerical weather prediction models were integrated both by the conventional grid-point method and by the spectral method proposed by Silberman (1954).⁸ For integrations spanning a hemisphere (or sphere) and for comparable space truncation measured in terms of phase speeds, the spectral method was found to be about twice as efficient in terms of computation time on the IBM 7094. Also, it eliminates the cascade of energy into the smallest resolvable scales and, compared with most grid-point methods, it is far superior in preserving the quadratic integral invariants of the differential equations. The latter is clearly depicted in Fig. 12. This shows results from comparable (one-hour time step

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⁷C. E. Leith, "Numerical Simulation of the Earth's Atmosphere," UCRL 7986-T.

⁸I. Silberman, "Planetary Waves in the Atmosphere," J. Meteor. 11, 27-34 (1954).

Fig. 12. Evolution of quadratic integral invariants during grid-point and spectral integration.

in each) grid-point (1977 data points) and spectral (333 expansion coefficients) integrations of the free-surface barotropic equation

$$(\nabla^2 - \kappa^2) \frac{\partial \psi}{\partial t} = -J(\psi, \nabla^2 \psi + f), \quad (1)$$

where $\psi \equiv$ stream function, $f \equiv$ coriolis parameter, and $\kappa^2 \equiv$ constant.

For each integration Fig. 12 shows the time variations of the mean squared vorticity (MSV), kinetic energy (KE), potential energy (PE) and the quadratic integral vorticity ($MSV + \kappa^2 KE$) and energy ($KE + PE$) invariants of Eq. (1). The grid-point integration, due to space truncation of finite differencing, is preferentially damping the smaller scale components. The resulting energy loss is most apparent in the loss of mean-squared vorticity which is most dependent upon the amplitudes of the small-scale components.

The only discovered disadvantages of the spectral method arise if tendency terms are multiplied by space-dependent variables, or if forcing terms are more than quadratic in space variables. In the former case tendency equations for the expansion coefficients cannot be uncoupled; this requires inversion of a matrix each time step and in the latter case, higher-order interactions occur which complicate the integration. These difficulties can be circumvented by replacing undifferentiated space variables by their mean values or by use of a primitive equation model in which such terms do not occur.

To provide initial data for these comparative integrations, IBM 7094 computer programs were developed to interpolate objective analyses (prepared by the National Meteorological Center at Suitland, Maryland) to a latitude-longitude grid and to compute surface spherical harmonic expansion coefficients from the interpolated data.

The initial report on this investigation is contained in Ellsaesser (1964).⁹ Comparative integrations of the baroclinic (two-level) model are now underway.

H. W. Ellsaesser

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⁹H. W. Ellsaesser, "Evaluation of Spectral versus Grid Methods of Hemispheric Numerical Weather Prediction," UCRL-7865-T (1964).

Propagation of Water Waves on Sloping Beaches

Calculations of the ratio of breaking depth to initial depth vs the ratio of initial amplitude to initial depth and the ratio of breaking amplitude to initial amplitude vs the ratio of initial amplitude to initial depth from Packham's¹⁰ results on solitary waves agree very well with the theoretical curves¹¹ based on McCowan's work.¹² For very small slopes both theories give curves agreeing reasonably well with the experimental results published by Ippen and Kulin.¹¹ The two ratios above are plotted in Figs. 13 and 14, together with some theoretical and experimental results by Ippen and Kulin. Our results are derived from the assumption that the potential energy of the solitary wave is conserved as it propagates toward the shore. On approximating a long infinitesimal sinusoidal wave by a solitary wave and the conservation of potential energy, we are able to derive a formula relating the breaking depth of an incoming (toward shore) sinusoidal wave.

$$h_b \approx 0.45 \lambda_{\infty}^{1/3} a_{\infty}^{2/3}$$

$$a_b \approx 0.998 h_b$$

where

h_b = the depth at the breaking

a_b = the amplitude (from crest to trough) at the breaking

λ_{∞} = the wave length of the sinusoidal wave

a_{∞} = the amplitude (from crest to trough) of the sinusoidal wave.

For example, a wave of wavelength 10,000 ft and amplitude 2 ft will break at a depth of 15.2 ft and an amplitude of 15.2 ft.

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¹⁰B. A. Packham, "The Theory of Symmetrical Gravity Waves of Finite Amplitude, II." Proc. Roy. Soc. London, 213 238-249 (1952).

¹¹A. T. Ippen and C. Kulin, "The Shoaling and Breaking of the Solitary Wave," Conf. Coastal Engin. 5 27-47 (1954).

¹²J. McCowan, "On the Highest Wave of Permanent Type," Phil. Mag. 38 351-357 (1894).

Fig. 13. Breaking amplitude for water waves on sloping beaches.

Fig. 14. Breaking depth for water waves on sloping beaches.

The application of Davies'¹³ periodic waves of finite amplitude to the propagation of a train periodic waves over a sloping beach is being carried out. With a slight extension of Davies' results we can show, with some of our preliminary calculation, that the ratio of wavelength to depth increases as a train of waves propagate toward shore. The main task here is to calculate the values of the elliptic functions of complex argument. The final results should help us to predict the breaking of a train of periodic waves.

K. S. Yee

Atmospheric Code Development

A zonal two-dimensional weather calculation. LAM,¹⁴ the three-dimensional numerical simulation of the earth's atmosphere, has so many zones that it requires considerable time (approx. 80 sec.) to carry out one cycle which advances the atmospheric time 10 minutes. For this reason it was felt that it would be useful to have an admittedly more crude but faster-running code. Such a calculation which would advance atmospheric time many days for each hour of machine time would be most useful in studying the effects of changes in calculation schemes and initial data.

A code ZAM which is particularly suitable for these purposes is obtained by considering the variables in LAM to be independent of longitude. The equations used for the numerical calculations minus their longitudinal structure can then be carried over directly from LAM. ZAM is able to exhibit the zonal nature of the atmospheric flow while still possessing a vertical and meridional structure capable of showing the cells which are observed in the real atmosphere. Being a two-dimensional code, ZAM has a one-zone belt in place of the 72 zones which exist at each latitude and pressure level in LAM, with a corresponding increase in computational speed.

At present ZAM is a most useful tool in the search for such things as more realistic small-scale convection schemes. In the future it can be used

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¹³T. V. Davies, "Gravity Waves of Finite Amplitude III." Quarterly Appl. Math. 10, 57-67 (1952).

¹⁴C. E. Leith, "Numerical Simulation of the Earth's Atmosphere," UCRL 7986-T.

to study the gross effects of changes in initial data, particularly in convection, with problems being carried out later on the full three-dimensional versions.

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J. J. Walton

Atmospheric model in FORTRAN. FLAM, a numerical model of the earth's atmosphere, is the FORTRAN version of the LAM¹⁴ code. In this model the state of the atmosphere — as specified by the temperature, specific humidity, wind velocity, and surface pressure — is defined as a three-dimensional grid covering the space surrounding the earth to a level of 50 mbars. Using the same equations as in the LAM code, the model predicts successive atmospheric states at 10-minute intervals.

The advancement from one state to the next requires two different calculational sweeps through the entire grid. During the first sweep the horizontal advection and diffusion of the state variables is accomplished in two steps: first the north-south advection and diffusion, the results of which are then used in the second step which is the east-west advection and diffusion. Using these results, the second sweep performs the incrementation of the state variables resulting from vertical advection and diffusion and the effect of the various thermodynamic forcing functions. The entire two-sweep cycle required to advance the state over one 10-minute interval takes the FLAM code 90 seconds on the CDC 3600 computer, whereas the LAM code takes only 61 seconds on the LARC.

Due to memory limitations, only a portion of the state variables are in the memory at any one time; the remainder are maintained in some less accessible storage units. On the CDC 3600 this latter storage consists of tapes; on the LARC, it consists of magnetic drums. Variables must be transmitted from these units to the memory before they are needed in the calculation.

Periodically the results of the calculation are edited to produce two-dimensional contour maps of zonal-averages of quantities such as temperature, specific humidity, and wind speeds. Other information concerning quantities such as latent heat release, convection, and the transport of various quantities in the atmosphere are also edited and displayed in the form of contour maps.

C. A. Sherman and R. J. McLean

RADIATION PHYSICS

Lasers and Plasma Physics

Stimulated Brillouin Scattering

The scattering of light by density fluctuations in matter has been the subject of investigation over a period of many years by a number of authors,^{1,3} and in particular by Brillouin,⁴ whose name the effect now bears. Recently the stimulated scattering of laser light by random acoustic waves in solids was observed by Townes and co-workers.⁵ Because of the accompanying production of acoustic energy, this effect presents a number of interesting implications. One is that a high-power laser constitutes a novel source of ultrasonic energy. Another is that the production and localized absorption of large amounts of acoustic power may constitute a damage mechanism affecting both laser media and transparent media used to transmit laser light.^{5,6}

Analyses of the stimulated scattering of light by acoustic waves, based on classical considerations, have been given by Townes *et al.*^{5,6} for the case of the scattered radiation and acoustic energy wholly contained within a resonant cavity and by Kroll⁷ for the traveling-wave case. These treatments assume the incident laser beam to be a monochromatic plane wave. In the present work the same question has been examined on the basis of a quantum theoretic approach. The justification for this approach in view of the applicability of classical methods is that it introduces the various stimulated processes in a very natural way, and it makes particularly simple the handling of cases wherein the incident laser beam is not a simple plane wave but is distributed in both frequency and direction.

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¹A. Einstein, Ann. Phys. 33, 1275 (1910).

²I. Tamm, Zeit. Phys. 60, 345 (1930).

³M. Leontowitsch and S. Mandelstam, Jr., Zeit. Phys. 75, 350 (1932).

⁴L. Brillouin, Ann. Phys. Paris 17, 88 (1922).

⁵R. Y. Chiao, C. H. Townes, and B. P. Stoicheff, Phys. Rev. Letters 12, 592 (1964).

⁶R. Y. Chiao, E. Garmire, and C. H. Townes, Proceedings of the Enrico Fermi International School of Physics, Course XXXI, 1963. To be published.

⁷N. M. Kroll, Bull. Am. Phys. Soc. 9, 222 (1964).

Both the acoustic and electromagnetic fields are represented in terms of normal modes which characterize the volume of the solid where the scattering takes place. The basis of the analysis is first-order perturbation theory which is used to derive Boltzmann equations for the phonon and scattered photon populations. Cross sections and rate constants have been obtained from these equations by summing over the modes represented respectively in the scattered and incident beams. The original results of Brillouin have been derived in succinct form, as have been the threshold conditions for the exponential buildup of the photon and phonon populations. Conditions (which depend on the power as well as the frequency and angular spread of the laser beam) have been derived for the exponential buildup of the scattered beam and associated phonons.

J. A. Fleck, Jr.
(UCRL-7968-T)

Laser Ion Source

The laser-induced production of plasma, and emission of ions, electrons, and neutrals has been studied recently at this Laboratory and elsewhere.⁸⁻¹⁷ As a result, the possibility of using a laser as a component of a high current heavy-ion source is being studied.

⁸G. Giori, L. A. MacKenzie and E. J. McKinney, "Laser Induced Thermionic Emission," Appl. Phys. Letters 3, 25 (1963).

⁹R. E. Honig, and J. R. Woolston, "Laser Induced Emission of Electrons, Ions, and Neutral Atoms from Solid Surfaces," Appl. Phys. Letters 2, 138 (1963).

¹⁰R. E. Honig, "Laser Induced Emission of Electrons and Positive Ions from Metals and Semiconductors," Appl. Phys. Letters 3, 8 (1963).

¹¹N. R. Isenor, "High Energy Ions from a Q-Switched Laser," Canad. J. Physics 42, 1413 (1964).

¹²N. R. Isenor, "Metal Ion Emission Velocity Dependence on Laser Giant Pulse Height," Appl. Phys. Letters 4, 152 (1964).

¹³D. Lichtman and J. F. Ready, "Laser Beam Induced Electron Emission," Phys. Rev. Letters 10, 342 (1963).

¹⁴W. I. Linlor, "Ion Energies Produced by Laser Giant Pulse," Appl. Phys. Letters 3, 210 (1963).

Fig. 15. Schematic drawing of test ion source.

In this Laboratory a Q-spoiled laser producing 0.2 J in 70 nsec has been used to produce a plasma at the surface of a nickel target. The plasma expands into contact with a nickel grid. A high positive voltage between the grid and the collector pushes the ions to the collector after they have leaked through the grid. With 3000 V between the grid and collector, an ion current of 14 A was measured by means of the 100- Ω monitor resistor and oscilloscope.

As a component of an ion source a laser presents several advantages: (1) the power to produce the ions can be delivered to relatively inaccessible areas in that only mirrors are needed, (2) the main power supplies remain external to any device using the ion source, and (3) any material that can be ionized by the laser may be used in the ion source. There is one disadvantage which as yet has not been overcome; there are no lasers producing enough

¹⁵W. I. Linlor, "Some Properties of Plasma Produced by Laser Giant Pulse," Phys. Rev. Letters 12, 383 (1964).

¹⁶J. F. Ready, "Development of Plume of Material Vaporized by Giant Pulse Laser," Appl. Phys. Letters 3, 11 (1963).

¹⁷C. M. Verber and A. H. Adelman, "Laser Induced Thermionic Emission," Appl. Phys. Letters 2, 220 (1963).

energy at a high enough repetition rate to produce ion pulses at the repetition rates obtained from current ion sources.

J. E. Swain

Thermonuclear and Neutron Physics

Vaidya's Radiating Schwarzschild Metric

The metric field surrounding a star, idealized as a radiating sphere, cannot be the Schwarzschild solution,¹⁸ except in the excellent approximation in which one neglects the energy density of the emitted radiation. In this work we have investigated the metric outside a spherically symmetric body when radiation is included. For a normal star, the influence of radiation on the metric is negligible when compared with the effects of deviations from spherical symmetry, caused by rotation, magnetic fields, etc.¹⁹ Nevertheless, this metric may have some relevance to the study of a collapsing supernova core,²⁰ if one allows for the production of a copious supply of neutrinos, but neglects their subsequent absorption in the outer envelope. A realistic treatment must, of course, analyze the problem of neutrino transport in detail. The solution described here is thus chiefly useful as an extreme limiting case, in which the neutrino optical depth of the envelope is negligible.

We therefore seek a spherically symmetric solution of the Einstein equations²¹

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¹⁸K. Schwarzschild, Sitzber, Preuss. Akad. Wiss. Physik-Math. Kl. 189 (1916).

¹⁹A metric for empty space surrounding a rotating object has been given by R. Kerr, Phys. Rev. Letters 11, 237 (1963). The asymptotic form had been obtained previously by A. Papapetrou, Proc. Roy. Irish Acad. A52, 11 (1948). Static metrics for empty space surrounding objects with axial symmetry were given by H. Weyl, Ann. Phys. 54, 117 (1917) and 59, 185 (1919) and have been further studied by M. Misra, Proc. Nat. Inst. India A26, 673 (1960) and A27, 373 (1961); G. Erez and N. Rosen, Bull. Res. Council of Israel 8F, 47 (1959); D. Zipoy, preprint, 1964.

²⁰S. A. Colgate and R. W. White, UCRL 7777 (1964).

²¹Throughout this paper we choose units such that $G = 1$, $c = 1$.

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi T_{\mu\nu}$$

with the "geometrical optics" stress-energy tensor of radiation

$$T^{\mu\nu} = qk^{\mu}k^{\nu}$$

in which k^{μ} is a null vector directed radially outward.

This problem has been considered by Vaidya,²² Raychaudhuri,²³ and Israel.²⁴ In Vaidya's metric for a radiating sphere,²⁵

$$ds^2 = - (1 - 2mr^{-1})du^2 - 2dudr + r^2 d\Omega^2$$

(where $m(u)$ is a nonincreasing function of the retarded time $u = t - r$) we verify that $-dm/du$ is the total power output as given by the Landau-Lifshitz stress-energy pseudo-tensor, and relate it through red shift and Doppler shift factors to the apparent luminosity L for an observer moving radially in this gravitational field. We argue that the hypersurface $r = 2m(u)$ cannot be realized physically, but see that a hypersurface $r = 2m(\infty)$ at $u = \infty$ (which is not adequately represented in presently available coordinate systems) shows the total redshift characteristic of the Schwarzschild "singularity." The geodesic equations are written out to display a gravitational "induction field" $GL/c^3 r$ associated with a changing mass in the Newtonian $-Gm/r^2$ field.

R. W. Lindquist, R. A. Schwartz and C. W. Misner*
(UCRL-12059-T)

Generation of Einstein's Field Equations by Computer

Some effort is being expended in the physics community in finding solutions of Einstein's field equations for general relativity. Since there is no general algorithmic procedure for doing this, the usual approach is to assume a form for the metric tensor involving one or more undetermined

²²P. C. Vaidya, Proc. Indian Acad. Sci. A33, 264 (1951). Curr. Science 21, 96 (1952).

²³A. K. Raychaudhuri, Z. Phys. 135, 225 (1953).

²⁴W. Israel, Proc. Roy. Soc. London A248, 404 (1958).

²⁵P. C. Vaidya, Nature 171, 260 (1953). We thank Prof. D. Zipoy for pointing out this work to us.

*Department of Physics and Astronomy, University of Maryland.

functions. The Einstein equations are then generated by computing the Einstein tensor corresponding to this assumed metric tensor. If the latter has been happily chosen, the equations are solvable.

A large fraction of the expended effort is involved in the calculation of the Einstein tensor once the metric tensor has been decided upon, a procedure which is entirely algorithmic but extremely tedious and offering considerable opportunity for careless error. A similar calculation must also be performed if the Einstein equations are to be prepared for numerical integration by computer, an area in which work is now being pursued at this Laboratory. Therefore, there is now under development at this Laboratory a computer program for generating Einstein tensors from given metric tensors.

The input to this program is a number giving the dimension of the problem (4, for relatively applications), the names of the coordinates (e. g., X, Y, Z, T), and algebraic expressions for the nonredundant components of the covariant metric tensor. The output consists of algebraic expressions for the nonredundant components of the contravariant metric tensor, the determinant of the metric tensor, the Christoffel symbols of the second kind, the Riemann curvature tensor, the Ricci and Einstein tensors, and the curvature scalar. The program is written in the LISP language and is now usable. Possible further refinements would be to include the ability to interpret arbitrary tensor-notation expressions and to allow FORTRAN-like formats for input-output rather than the present LISP prefix notation.

J. G. Fletcher

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