NUCLEAR EXCITATIONS AND REACTION MECHANISMS

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ABSTRACT

A. (Fallieros). The nuclear Compton amplitude, dispersion relations, model calculations, electroexcitation sum rules, effects of nucleon size on photonuclear transitions and internal nucleon excitations.

B. (Levin). Wave function formalisms in the channel coupling array theory, test of bound state approximations, new n-particle scattering theory, atomic and molecular bound state calculations.

C. (Li). Test of bound state approximations in many-body scattering theories, quantum theory for nonhermitian operators, and variational principles for particles and fields in Heisenberg matrix mechanics.
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Scope</td>
<td>1</td>
</tr>
<tr>
<td>2. Current Research</td>
<td></td>
</tr>
<tr>
<td>A. (Professor S. Fallieros)</td>
<td>2</td>
</tr>
<tr>
<td>B. (Professor F. S. Levin)</td>
<td>8</td>
</tr>
<tr>
<td>C. (Dr. G. T. Li)</td>
<td>14</td>
</tr>
<tr>
<td>3. Other Activities</td>
<td>20</td>
</tr>
<tr>
<td>4. Personnel</td>
<td>22</td>
</tr>
<tr>
<td>5. Year's Publications</td>
<td>23</td>
</tr>
</tbody>
</table>
SCOPE

The nuclear physics group at Brown University has continued to comprise five physicists, two faculty members in experimental physics and the two faculty members and one Research Associate engaged in theoretical research. As in the past, the collaboration between experimentalists and theorists continues.

This progress report contains in the three parts, A, B, and C, the descriptions of the work of Professors Fallieros and Levin and of Dr. Li. Research is carried out in the Barus and Holley Physics-Engineering Building while numerical analyses have been done at Brown on the IBM System 360/67.
The nuclear Compton amplitude and dispersion relations.

This is a continuation of work partially described in last year's report. We have obtained a twice-subtracted dispersion relation which has a number of advantages over the more conventional expressions of the standard Kramers-Kronig type: (a) as emphasized in previous discussions the standard relations are not valid for non-relativistic systems except in the simple case of purely electric dipole transitions. Since the prediction and the interpretation of experimental results is always made in terms of non-relativistic nuclear models, it is important to have an approach which minimizes this inadequacy. The second subtraction was meant to do that and it has now been verified that the consistency of this approach is quite satisfactory even when electric quadrupole and other transitions are important. (b) the dispersion integrals can only be evaluated up to energies available to experiments. The approach we are considering has decreased the error originating from the unavoidable finiteness of the upper limit in the dispersion integral. (c) advantage is taken of the existence of rigorous theoretical expressions for the slope of the scattering amplitude at low energies as well as of the availability of experimental results for this expression. Since these results come from the experiments that measure the dispersion integrals, the scheme has an appealing consistency and reliability.

We have, in addition, studied the angular distribution of the scattered radiation. The subtraction terms are known to be of purely dipole character.
(both electric and magnetic) and it was properly verified that the quadrupole contributions appear only at higher energies. Although this is expected by rather general arguments, the application of somewhat inconsistent approaches was seen to violate this expectation. We have also tried to emphasize the importance of polarization measurements of scattered photons in the energy region \( \sim 20 - 50 \text{ MeV} \). These should make possible the separation of e.g., the nuclear polarizability into its electric and magnetic parts. The polarizability is known experimentally in many nuclei, but this quantity is expected to be dominated by its electric-dipole component. Our experimental knowledge of magnetic excitations is very limited and any information on the magnetic strength in the energy region mentioned above should be important.

**Exact calculation of the photon-scattering amplitude for a simple system.**

This work has now been completed and is described in the first part of Dr. C. Ercil's Ph.D. thesis. It is currently being prepared for publication. A number of new items has been added to what was already reported in last year's progress report; some of them will be mentioned below. The intention of this work was to simplify the target of a photon-nucleus experiment and obtain complete analytic results for transition amplitudes that are essentially impossible to calculate in a more realistic situation. The target was limited to single-particle excitations and harmonic-oscillator wave functions were used for all states involved. The results have already been found useful, serving as models or limits for the more complicated photon-induced transitions that we have been studying. All possible multipolarities and all degrees of retardation have been included and the
photons have been allowed to be either real (on the mass shell) or virtual. Among the results we mention a test of the validity of a method often used in the literature for the evaluation of retardation in electric-dipole transitions. It was found that a term normally neglected in such calculations is really of the same order as what is calculated. A correction of essentially a factor two is what is indicated by our new estimates. In addition to its unexpectedly large magnitude this term is significant because it is not part of what is contained in the results of Siegert's theorem. This implies that mesonic corrections are needed here and might become quite important when the photon wavelength becomes equal to or smaller than the nuclear radius.

The results of this work were used also to test the validity of the Kramers-Kronig dispersion relations for a simple non-relativistic system. In accordance with our previous work, it was found that these relations were indeed not satisfied by our system. In this case, however, we are able to estimate the necessary corrections to any desired order of retardation. Since these results were summarized in terms of simple physical quantities (e.g. nuclear size, multipolarity of the transitions, etc.) they can be used as a reasonable guide in situations where the calculation of such corrections is not possible.

A study has also been made of possible zeros or at least minima in the photon-scattering amplitude. Although the problem is clearly defined in a situation where the target contains only discreet energy levels it seems to become less meaningful for a nuclear target where the excitation spectrum after a certain energy becomes continuous. Our interest in this
question was, however, motivated by a consideration of a doorway type of structure in the target, e.g., a situation where two basic collective states are providing the dominant response of the target to the external probe.

**Electroexcitation sum rules for transverse nuclear currents.**

We have developed a number of energy-weighted sum rules for single-particle transitions induced by transverse currents associated with virtual photons. The limitation to one-body transitions is at this point essential; work concerned with the many-body situation is anticipated and will be described in this year's research proposal. Some of our results are general i.e., independent of the detailed nature of the single-particle wave functions while others consist of detailed calculations and representative graphs for selected specific cases. Among the more general results, we mention a theorem concerning the functional dependence of the right-hand side of the sum rule on the momentum, \( \overrightarrow{q} \), of the virtual photon: for a sum rule containing the \( n \)th power (with \( n \) positive) of the excitation energy of the target, the right-hand side is a polynomial in \( \overrightarrow{q}^2 \) with maximum power equal to \( n \). The origin of this statement has been traced to the local nature of the equal time commutator between the current and the charge density of the system, i.e. the fact that it vanishes when these two quantities are taken at different points in space. Since the current operator contains derivatives which do not commute the potential energy of the system, sum rules involving this quantity are more complicated than those related to just the transition density of the system. General re-
strictions of the type mentioned above become then more important since often the exact structure of the sum is difficult to predict in detail.

The theorem stated above is not valid for sum rules containing negative powers of the excitation energy. For such cases, we have performed detailed calculations for specific situations. We have also related the results to the high-energy behavior of the virtual scattering amplitude and connected the results to the properties of the transverse response function of the system under consideration.

Nucleon size, photnuclear transitions and nucleon excitations.

This work overlaps with the second part of Dr. C. Ercil's Ph.D. thesis whose completion took somewhat longer than we originally anticipated. The investigation is now finished and a manuscript summarizing its main results is in preparation. Dr. Ercil has returned to his country (Turkey) and is employed at the Middle East Technical University.

The basic model used for this study was already described a year ago. It was constructed with the intention of avoiding an ad hoc introduction of internal nucleon degrees of freedom. All nucleon size and internal nucleon excitation effects appear simply as a result of the binding of point particles creating a composite system which in turn, makes transitions associated with the absorption or emission of photons. Among the problems that we have studied using this model we mention the question concerning the possible energy dependence of the forward amplitude describing contact, two-photon interactions. In an ordinary nuclear-physics problem such energy dependence arises from the introduction of the in-
trinsic nucleon form factor and/or from contributions describing mesonic charge exchange. We have shown that if such effects are introduced without any additional modifications of the theory, inconsistencies appear which tend to become quite significant when the photon wavelength becomes comparable to the pion Compton wavelength. In the model we are considering, however, such effects are not introduced by hand but follow from the detailed development of the theory. The complete forward amplitude has no energy dependence at all, but contains components with energy dependent terms which just cancel each other when the sum is taken.

The model we have developed has been noted to have some interesting analogies with what takes place in the Mössbauer effect; the nucleus in this effect is now replaced by a nucleon while the phonon excitations are in our case the excitations of the low-lying nuclear states.
Wave function formalisms in the channel coupling array theory

Work on this topic, noted in last year's Renewal Proposal, is now complete, and an article based on it has been written and submitted to Physical Review C for publication. Several new results are contained in this paper, which is briefly summarized in the following.

One may generally classify the scattering formalisms obtained via channel coupling array (CCA) procedures into two categories, which, following the nomenclature of Tobocman, are denoted the Kouri-Levin (K-L) and the Baer-Kouri (B-K) classes. From the transition operator equations of each of these classes one concludes that they are quite different in meaning and structure, and this has been verified by means of various approximate calculations. The description based on equivalent wave function formalisms illustrates this difference in explicit detail and provides a new and easily understandable explanation for the occurrence of non-unitary amplitudes in approximate calculations based on the B-K operator equations as found by Baer and Kouri and by Lewanski and Tobocman. The basic idea is to express the equivalent wave function formalism as a set of differential rather than integral equations. In such form, the K-L equations are found to be homogeneous, so that approximations to them will be flux-conserving, i.e., unitary, as has been found numerically. On the other hand, the differential form taken by the B-K wave function equations are inhomogeneous and, as was shown some time ago by Dahlgren and Levin, approximations to inhomogeneous scattering equations will almost certainly lead to non-unitary (even a-causal) amplitudes. The non-unitary character of the approximate B-K calculations is thus now seen to be a not-unexpected consequence of the structure of the B-K equations; this renders them less useful than had been considered heretofore.
Test of the bound state approximation

Calculations designed to test the use of bound state approximations (BSA's) using a very simple 3-body model were described in last year's Progress Report and additional ones were proposed in the Renewal Proposal for the current contract year. The new calculations were to be done using an IBM version of the Doleschall 3-body code, to have been obtained from J. P. Svenne in Manitoba, with Dr. Li mainly responsible for the details of this work. Prof. Svenne did send the code and the task of making it run on the Brown University IBM computer, which occupied a number of months of Dr. Li's time, seems more or less complete. Calculations for a variety of one-particle-transfer reaction models are now being carried out. These have a double purpose: first to provide exact results against which to compare the BSA results, and second to examine details of (d,p) and (p,d) reactions within an exact model that have not been previously studied, such as the role of coupling to several bound states in other channels; the effect of capture into non 1 = 0 orbits, and the coupling interference between orbits of different l in the same channel.

In addition to the Doleschall code obtained from Prof. Svenne, another very useful computer code has very recently been received: the CRC code developed by R. D. Koshel and his students. The task of making this new code compatible with the Brown IBM computer is in progress. This code will also play an important role in our bound state calculations as described in the Renewal Proposal.

A final point with respect to the BSA work concerns a longer paper on the first calculations, recently published with J. M. Greben in Physical Review C. In addition to providing more detail than is found in the Physical
Review Letters paper, the longer article presents arguments explaining the agreement at low energies and forward angles and the disagreement at higher energies and larger angles between the exact and BSA results. The analysis is based on the behavior of the nearest singularity (dominant pole term) in the amplitude.

**New n-particle scattering theory**

There are two classes of transition operators and corresponding wave function components that have so far been derived using the channel coupling array (CCA) $W$. The channel permuting array (CPA) choice of $W$ leads to a general class of equations valid for arbitrary numbers of particles $n$. There are, however, certain problems associated with the CPA class, as noted below. The second class of theories has been obtained using a Faddeev-Lovelace (F-L) choice of $W$. These have been much less general than the CPA choice. Originally only two sets of equations for the $n = 3$ case were obtained.

In wave function form, one set lead to the Faddeev wave function component equations, while the other lead to a set in which the "components" were each equal to the exact scattering solution of the Schrödinger equation. (A similar division into "true" components and "components" which are each equal to the full scattering wave function is also found with the CPA choice of $W$.)

Several years ago, an extension from the $n = 3$ F-L case to arbitrary $n$ was made, in connection with studies of the Bencze-Redish-Sloane (BRS) formalism. In particular, it was found possible to derive the so-called precursor form of the BRS equations using an F-L choice of $W$. The corresponding wave function formalism was of the second type noted above, which is much less useful than a formalism based on true components. A search for a generalized
(arbitrary n) form of F-L equations involving true components has been ongoing for some time. Due to the complexity of the analysis, the problem of extending the Faddeev-type components from the 3-body case to the arbitrary n-particle case had eluded solution. This problem has now been solved, providing a new and what at present seems likely to be an important addition to the family of many-body scattering theories.

The new theory combines techniques from the CCA and BRS formalisms to produce transition operators with equivalent, true wave function components. Both transition operators and wave function components are treated symmetrically in the equations they obey, as opposed to the a-symmetric formulation of the CPA-based equations. The new equations are defined in terms of partitions, thus allowing for treatment of particle identity in a simple linear fashion, along the lines discussed by Bencze and Redish. That is, the new operators and components are label-transforming, unlike the CPA operators which have been so troublesome to symmetrize in the past. (In effect, by introducing the new formalism, the problem of exchange effects noted in last year's Renewal Proposal has now been satisfactorily solved within the general CCA formalism, although not for a CPA set of operators or wave functions. It now appears to be a certainty that no antisymmetrization procedure for the CPA theory exists that does not employ an iteration of the equations, thus making them rather more complicated to solve than in non-iterated form.)

The new theory has a structure somewhat similar to that of the precursor BRS formalism, although in contrast to this latter formalism the new one yields true wave function components. For both the new transition operator and wave function equations, one can perform the summations over those partitions containing three and more clusters to derive minimal sets of equations,
i.e., sets in which only the 2-cluster partitions occur, in precise analogy to the BRS scheme. When the scattering system contains three particles, the wave function component equations reduce to the original Faddeev equations.

The new theory appears to be a rich lode to mine, and some relevant future research is noted in the accompanying Renewal Proposal. An article outlining the derivation of the new theory is in preparation.

Atomic and molecular bound state calculations

Calculations designed to test the convergence of basis expansions in the CCA procedure, for atomic and molecular bound states, as proposed in last year's Renewal Proposal, have been carried out by W. Ford. Although the H₂ molecule was initially chosen as the system to be examined, it was subsequently decided to test various approaches for the simpler molecule H₂⁺. Computation corresponding to two basis set expansions have been performed. In the first, pure hydrogenic (bound) states have been used. The resulting H₂⁺ ground state energies were found to oscillate with increasing basis size and no indications of convergence to the correct answer were found. This was not surprising given the oscillatory nature of the analogous H⁻ calculations done some years ago by J. Chen and collaborators using the Faddeev equations and bases consisting of both hydrogenic and of Sturmian functions. In addition, there is the much older result of Shull and Löwdin on the need to include continuum states when a hydrogenic expansion basis is used. To circumvent this problem, Shull and Löwdin introduced another basis set, similar to the hydrogenic basis, but containing only bound-state-type functions, in analogy to the harmonic oscillator basis. The second set of H₂⁺ calculations was therefore performed using the Shull-Löwdin basis. The results were generally the same as found in the previous calculations: oscillatory behavior.
and lack of convergence to the known $H_2^+$ ground state energy.

This behavior seems now to be characteristic of basis set expansions for CCA-type bound state calculations involving Coulomb interactions. Such expansion methods for determining eigenstates and eigenvalues of an arbitrary linear operator are collectively known as Galerkin (or Bubnov-Galerkin) methods. General theorems lead one to expect eventual convergence although not monotonically. Rather than attempt to find convergence through a series of larger and larger basis expansion calculations, whose efficacy is not assumed in advance, it was decided to employ an entirely different procedure, viz, the finite element method, well known in engineering applications but apparently not very much used in physics computations. This is a numerically quick and, if the engineering applications are taken as a valid guide, rapidly converging procedure to use. Mr. Ford is currently engaged in the details of the finite-element computations.

**Other research**

In addition to the preceding, work has continued on most of the other topics noted in last year's Renewal Proposal, such as dispersion-theoretic approaches to many-body scattering, quantum theory for non-hermitian operators, and spectral properties of non-hermitian operators (Dr. Li has obtained some interesting results for a non-hermitian, non-linear oscillator problem, as noted in section 2C). There is no significant progress to report on here, and work is simply expected to continue on these topics.
Test of Bound State Approximations

Calculations designed to test the use of bound state approximations for various 3-body models more sophisticated than the one used in last year's calculations are now in good progress. For the purpose of these calculations we are using an IBM version of the 3-body code written by P. Doleschall as well as the CRC code developed by R. D. Koshel and his students. Both of these codes have now been properly altered to run on the Brown University computer system. This includes test runs designed to reproduce some existing results from previous calculations using other numerical methods. In the case of the Doleschall 3-body code, these test runs enabled us to discover and correct two minor but nontrivial errors in our copy of the code. In the case of the CRC code the technical difficulties caused by different computer systems have also been overcome.

Other details of research work on this topic in collaboration with Professor Levin have already been given in the preceding section of this progress report (Sec. 2B) and, therefore, will not be repeated here.

Quantum Theory for Non-hermitian Operators

Although work on this topic has no significant progress in its original direction noted in last year's proposal, it has inspired an investigation into another interesting non-hermitian operator problem occurring in high energy scattering theories, i.e. Reggeon field theory in zero transverse dimensions (Reggeon quantum mechanics).
Reggeon field theory (RFT) is a field theory formulated on a two-dimensional transverse space defined by the impact parameter and with a "time" variable which is actually the rapidity of the scattering process. Essentially, RFT is an extension of the earlier ideas of Regge poles and Regge cuts successfully introduced into elementary particle physics. In the last few years it has been developed into a powerful tool for analyzing the complex angular momentum structure of high energy scattering amplitudes. For the theory to make sense it is essential that the RFT Hamiltonian be non-hermitian. However, this non-hermitian Hamiltonian is also a source of mathematical troubles which have persistently impeded our full understanding of the theory.

Under appropriate approximations RFT can be effectively reduced to zero transverse dimensions. This simplifies RFT to only a one-dimensional quantum mechanical problem, i.e. Reggeon quantum mechanics (RQM). Recently, the study of RQM has made significant contributions to our understanding of the theory, in higher transverse dimensions. Besides, RQM also serves as a theoretical laboratory for testing various approximation techniques used for the general theory. However, owing to the fact that the Hamiltonian is non-hermitian, most of the standard techniques for hermitian operator problems are not applicable to RQM.

The purpose of the present investigation was to develop a practical and accurate calculation scheme for the energy eigenvalues and various matrix elements in RQM. The approach we use here is based on Heisenberg's matrix mechanics and the method of spectral decomposition. Previously we have applied this approach successfully to one-dimensional anharmonic oscillators.
As shown by the calculations carried out for the RQM system with triple-pomeron couplings, this approach also proves to be very practical for the present non-hermitian operator problem. In fact there is a strong similarity between the RQM system with triple-pomeron couplings and the one-dimensional anharmonic oscillator with quartic anharmonicity. Namely, the two systems possess harmonic spectra in one limit and resemble a degenerative double-well potential problem in another. In both of these limits the present approach not only provides one with an accurate numerical calculation scheme but also allows one to do analytic analyses for the spectral structures of the systems. This is one of the advantages of the present approach over the recursion-relation approach applied to RQM by R. Blankenbeckler and R. K. Sugar. This latter method is especially efficient for evaluating the energy eigenvalues and the Green's functions (but not the various matrix elements). However, it is difficult to adapt to the analytic analyses described above, if not impossible.

In the present approach one evaluates the matrix elements of products of operators by using the spectral decomposition and approximates the intermediate sums by only a finite number of terms. This is possible in the case of one-dimensional anharmonic oscillators because \( <n|a|n'> \) and \( <n|a^+|n'> \), the matrix elements of the annihilation and creation operators between exact eigenstates of the Hamiltonian, fall off rapidly as the difference \( |n-n'| \) gets large. In the case of ROM, because of the symmetry properties of the non-hermitian Hamiltonian, the corresponding matrix elements \( <n_L^*|a|n_R'> \) and \( <n_L^*|a^+|n_R'> \) of the annihilation and creation operators between exact left-hand and right-hand eigenstates alternate in value between pure real and pure
imaginary as \( n \) or \( n' \) is varied. Thus, what is a sum of all positive terms in the case of anharmonic oscillators can become a sum of terms alternating in sign. This makes the matrix elements

\[
\langle n_L | a^+ | n_R' \rangle \quad \text{and} \quad \langle n_L' | a | n_R \rangle
\]

with \( n' > n \) fall off very slowly as \( n' - n \) gets large. However, as can be shown, the specific structure of the system still requires that the other half of the matrix elements of \( a \) and \( a^+ \), i.e.

\[
\langle n_L | a | n' \rangle \quad \text{and} \quad \langle n_L' | a^+ | n_R \rangle \quad \text{with} \quad n' < n,
\]

should decrease rapidly in magnitude as \( n - n' \) gets large. Fortunately, having good fall-off properties for only this latter half of the matrix elements is sufficient for the present approach to be applicable. In fact, successive orders of approximation as obtained by keeping more and more intermediate states in the sum rules converge almost as rapidly as in the case of anharmonic oscillators. An article on this work is currently in preparation.

Variational Principles for Particles and Fields in Heisenberg Matrix Mechanics

Work on this topic has been done in collaboration with Professor Abraham Klein of the University of Pennsylvania and Dr. Moyes Vassanji of Chalk River Nuclear Laboratories (Ontario, Canada). An article based on it has been written and submitted to the Journal of Mathematical Physics for publication. Following is a summary of the main content in this paper.

A special calculational scheme useful in a wide class of problems in quantum mechanics and the many-body problem emerges from Heisenberg's matrix mechanics when matrix elements of products of elementary operators appearing in equations of motion and in commutation relations are evaluated by physically
chosen approximations to the completeness relation (sum over intermediate states). This calculational method, first introduced for the study of nuclear collective motion, has been applied in recent years to problems in particle quantum mechanics and solitons in quantum field theory. Although the fact that the formulation of this method possesses a variational content has been sporadically discussed or alluded to, this content has never been systematically and thoroughly explored. The purpose of this paper is, therefore, to present a series of variational principles based on Heisenberg’s matrix mechanics for a range of systems from one-dimensional quantum mechanics to quantum fields.

The unifying aspect in this variational approach is the construction of a stationary expression in which the variational parameters are matrix elements (ultimately between energy eigenstates) of the elementary operators of the theory. In particle quantum mechanics these are the $x$'s and $p$'s, in field theory the particle creation and annihilation operators. For each case surveyed, it is demonstrated that the appropriate stationary expression is the trace of the Hamiltonian over the space of states studied, subject to constraints which remind one that the variations of the $x$'s and $p$'s or their equivalents are restricted by their commutation relations. The structure of the variational principle suggests that the natural setting for this approach is indeed that class of problems where the need is to characterize the properties of a special band of states selected from a much larger space (as opposed to a single state).

Besides the applications to one-dimensional quantum mechanics and
and many-particle quantum mechanics, this variational approach is also applied to non-relativistic field theories for bosons and fermions. For these field theories, variational principles in which matrix elements of the density operators are chosen as fundamental variational principles for the density operators are new results which generalize known results from Hartree-Fock theory.
OTHER ACTIVITIES

The following invited lectures were given by members of the group:

"Some Aspects of Multistep and Breakup Effects in Light-Ion Induced Reactions" (F. S. Levin, University of Montreal, March 1979).


"Electric Dipoles" (S. Fallieros, University of Montreal, Feb. 1979).

"Nucleon Excitations and Photoneuclear Reactions" (S. Fallieros, McGill University, Feb. 1979).

"Fundamentals of Photoneuclear Physics" (S. Fallieros, Rutgers University, March 1979).

The Few-Body Gordon Conference ended on 17 August 1979 and on 20 and 21 August the second post-Gordon-Conference workshop on many-body scattering theory was organized at Brown University by Professor Levin. In attendance were E. O. Alt, W. Glückle, H. Haberzettl and W. Sandhas
from West Germany and C. Chandler, J. Evans, A. Gibson, R. Goldflam, D. Hoffman, K. Kowalski, T. Lim, and W. Tobocman from the USA. Funding, consisting of two or three nights' accommodation at a Brown University dormitory plus two day's per diem, was provided for the German visitors and those U.S. participants without direct contract support, i.e., all U.S. visitors but Hoffman, Kowalski and Tobocman. The workshop was extremely successful, with talks given by Chandler, Evans, Goldflam, Sandhas and Tobocman, with considerable discussion during and after the presentations. Since there was no line item for the workshop in the current budget, the funds were taken from the previously unexpended funds earmarked for Professor Fallieros' (cancelled) trip to the Mainz meeting. It is our plan to hold such workshops following future (bi-annual) Few-Body Conferences, funding for which will be included in the relevant budgets.
PERSONNEL

Professor S. Fallieres
Professor F. S. Levin
Research Associate Dr. C. T. Li
Research Assistant W. Ford
YEAR'S PUBLICATIONS


7. "Nucleon Form Factors and Nucleon Excitations in Nuclear Electromagnetic Transitions" (with C. Ercil and J. L. Friar), to be published.


9. "Nonlinear Generalization of the Quasiparticle Random Phase Approximation for Description of Anharmonic Effects in Vibrational Nuclei; Method"
YEAR'S PUBLICATION


