($<84°$). A normalization factor of 1.56 was required. This normalization was used for both the (d, d) and (d, p) distributions and is included in Figs. 7 and 8. When this absolute normalization factor is used, the present elastic results at back angles ($>90°$) are higher than those of Bassel *et al.* by about 25%, although the distributions agree well relatively at forward and backward angles separately. The present work used ten overlapping angles to determine the forward-to-backward normalization factor, which was found to be 1.018.

The results of the comparison of the ground-state distributions show good *relative* agreement over the entire angular range between the present data and the results of Kato *etal.* and Lee *et al.* However, while the present absolute cross sections and those of Kato *et al.* agree well (to within 10%), the absolute cross section of Lee *et al.* is about 25% larger than the present results. Further, the $E_d=11$ MeV absolute cross section of Lee *et al.* is about 25% higher than it might reasonably be expected to be with respect to their own $E_d=10$ MeV and $E_d=12$ MeV distributions. This discrepancy has been independently noted by Schwandt and Haeberli.[24]

Comparisons of the remaining (d, p) angular distributions at $E_d=11$ MeV are as follows: (a) The relative agreement of the 1.95-MeV distributions is good, but the absolute cross section of Lee *et al.* is about 25% higher than in this work, as was the case of the ground state. (b) The relative agreement of the 2.47-MeV distributions is good, but the absolute cross section of Lee *et al.* is higher than the present results by about 50%. (c) The relative agreement of the 3.95-MeV distributions is not as good as for the other distributions, and the absolute cross section of Lee *et al.* still seems to be 50% higher than obtained here. The larger difference between the absolute cross sections for the 2.47- and 3.95-MeV distributions as well as the poorer relative agreement for the 3.95-MeV distribution may be due to the presence of several lower-intensity proton groups associated with (d, p) reactions to neighboring states which were incompletely resolved.

[24] P. Schwandt and W. Haeberli, Nucl. Phys. **A123**, 401 (1969)

PHYSICAL REVIEW VOLUME 181, NUMBER 4 20 MAY 1969

Nuclear Energy Levels of V^{51}, Mn^{53}, and Co^{55} by the Quasiparticle Method

RAM RAJ, M. L. RUSTGI, AND R. P. SINGH
Physics Department, State University of New York, Buffalo, New York 14214
(Received 26 November 1968)

The modified Tamm-Dancoff approximation has been applied to the calculation of the nuclear energy levels of V^{51}, Mn^{53}, and Co^{55}. The shell-model reaction matrix elements of Kuo and Brown, calculated with the Hamada-Johnston nucleon-nucleon potential and renormalized for core polarization, are used with the aim of ascertaining the accuracy of these matrix elements. The effects of the extra term in the BCS equations and of the ground-state correlation are studied. Only a qualitative agreement between theoretical and experimental spectra is found for all three nuclei investigated.

1. INTRODUCTION

IN large measure, the degree of success in a shell-model calculation of the structure of a given nucleus depends on the degree to which the assumed closed core is really closed and on the residual interaction employed. Some of the difficulties found in shell-model calculations in which O^{16} and Ca^{40} are assumed to be closed cores come about because these nuclei are not really good closed cores.[1] There is some evidence that Ca^{48} forms a good closed core.[2,3] The conventional approach of assuming some simple but reasonable forms for the residual interaction has been questionable. An alternative approach is to treat the shell-model matrix elements themselves as adjustable parameters,[4] without specifying the algebraic forms of the interactions. This approach becomes futile because one has to decide beforehand which configurations should be included and which experimental levels are to be fitted. Yet there is a third approach, pursued by Kuo and Brown,[5] in which the effective interactions are deduced from the free nucleon-nucleon potential determined by the scattering data below the meson threshold. Two such potentials, which are known to be numerically similar, have been obtained by Breit and collaborators[6] and by Hamada and Johnston.[7]

Recently Kuo and Brown[5] have calculated the shell-

[1] G. E. Brown and A. M. Green, Nucl. Phys. **85**, 87 (1966).
[2] E. Kashy, A. Sperduto, H. A. Enge, and W. W. Buechner, Phys. Rev. **135**, B765 (1964).
[3] T. W. Conlon, B. F. Bayman, and E. Kashy, Phys. Rev. **144**, 940 (1966).
[4] P. Federman and I. Talmi, Phys. Letters **19**, 490 (1965).
[5] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **A114**, 241 (1968).
[6] K. E. Lassila, M. H. Hull, Jr., H. M. Ruppel, F. A. McDonald, and G. Breit, Phys. Rev. **126**, 881 (1962).
[7] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 382 (1962).

TABLE I. Values of E (MeV) and V. The column identification for each nucleus without and with term (5) is as follows: (1) E (MeV) and V values obtained from the solution of the BCS equations using the pairing matrix elements of Kuo and Brown; (2) the energy of the predominantly one-quasiparticle states obtained by the MTDA matrix diagonalization without ground-state correlation; (3) (for V^{51} only) the same quantity as in (2) but with ground-state correlation.

Nucleus	V^{51}						Mn^{53}				Co^{55}			
E (MeV) and	Without term (5)			With term (5)			Without term (5)		With term (5)		Without term (5)		With term (5)	
V	(1)	(2)	(3)	(1)	(2)	(3)	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)
$E_{1/2}$	7.48	6.51	6.52	7.80	6.86	6.86	6.77	5.77	7.13	6.16	5.80	4.98	6.33	5.78
$E_{3/2}$	4.99	4.77	4.77	5.30	5.11	5.11	4.28	3.93	4.64	4.28	3.33	2.83	3.84	3.38
$E_{5/2}$	6.69	6.35	6.36	6.95	6.65	6.65	6.02	5.62	6.36	5.99	4.98	4.60	5.54	5.24
$E_{7/2}$	1.57	1.42	1.45	1.55	1.43	1.45	1.65	1.43	1.67	1.45	1.87	1.58	2.33	2.12
$V_{1/2}$	0.086			0.072			0.107		0.098		0.111		0.112	
$V_{3/2}$	0.108			0.088			0.142		0.127		0.163		0.155	
$V_{5/2}$	0.154			0.130			0.183		0.173		0.181		0.188	
$V_{7/2}$	0.591			0.551			0.766		0.784		0.913		0.979	

model reaction matrix elements for the $0f$-$1p$ shell for the Hamada-Johnston nucleon-nucleon potential which are renormalized for the Ca^{40} core and Ca^{48} core. In their paper, Kuo and Brown pointed out that it is difficult to ascertain the accuracy of the calculated reaction matrix elements. Although they have given rather satisfactory results for some standard nuclear-structure calculations involving the interaction of two valence nucleons, they have certainly not tested the matrix elements severely enough. As a further test of these matrix elements, it is suggested that more extensive calculations be carried out, such as shell-model calculations involving the interaction of several nucleons which should be more sensitive to the individual matrix elements. It is in this spirit that the results on V^{51}, Mn^{53}, and Co^{55} are presented in the present paper.

Some authors[8] have made shell-model calculations on V^{51} and Mn^{53} assuming $(0f_{7/2})^3$ and $(0f_{7/2})^{-3}$ configurations for the protons, and that the neutrons form an inert core corresponding to the semimagic number 28. In deriving the reaction matrix elements using Ca^{48} core, Kuo and Brown used the $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ orbitals for the protons, just as we intend to do in this work. However, if the protons are assumed to be distributed in these orbitals, the shell-model calculation for Mn^{53} and Co^{55} become quite involved. But such calculations can still be easily carried out using the approximate quasiparticle method. It is assumed, following earlier works, that the interaction among these protons in the outermost partially filled shells gives rise to the observed spectra of these nuclei.

The modified Tamm-Dancoff approximation (MTDA) method, developed earlier[9] and extended recently,[10] has already been applied with success to odd Ni isotopes[11] and even Ni and Sn isotopes.[12] This method uses a complete set of orthonormal and nonredundant quasiparticle basis states and describes the levels of odd nuclei as a superposition of one- and three-quasiparticle states. In this paper the MTDA method is employed to calculate the energy-level spectra of V^{51}, Mn^{53}, and Co^{55} nuclei.

It is, however, interesting to note that a direct configuration-mixing calculation, without recourse to the approximate quasiparticle method, is quite feasible in V^{51}, which has three protons outside Ca^{48} core. Therefore, the results of the quasiparticle calculation on V^{51} can be checked against their exact shell-model results as a further test of the goodness of the approximation involved in the quasiparticle method.

In order to predict the detailed spectra of an odd nucleus by the quasiparticle method one has to mix one- and three-quasiparticle states. The detailed method of calculation and all working formulas are given in Ref. 9. Only some of the relevant formulas are given below for the purpose of particular interest. All the notations used here are defined in Refs. 9 and 11.

The chemical potential λ and the energy gap parameters Δ_a are obtained by solving the BCS equations

$$\Delta_a=\tfrac{1}{4}\sum_b([b]/[a])^{1/2}[G(aabbo)/E_b]\Delta_b \qquad (1)$$

and

$$N=\tfrac{1}{2}\sum_a[a][1-(\hat{\epsilon}_a-\lambda)/E_a]. \qquad (2)$$

[8] J. D. McCullen, B. F. Bayman, and L. Zamick, Phys. Rev. **134**, B513 (1964); A. de Shalit, in *Selected Topics in Nuclear Theory*, edited by F. Janouch (International Atomic Energy Agency, Vienna, 1963), p. 209.

[9] M. K. Pal, Y. K. Gambhir, and Ram Raj, Phys. Rev. **155**, 1144 (1967).

[10] Ram Raj and M. L. Rustgi, Phys. Rev. (to be published).

[11] Y. K. Gambhir, Ram Raj, and M. K. Pal, Phys. Rev. **162**, 1139 (1967).

[12] Ram Raj, Y. K. Gambhir, and M. K. Pal, Phys. Rev. **163**, 1004 (1967).

TABLE II. Energy levels (MeV) of V^{51} by the MTDA method. All the levels are relative with respect to the lowest level. Numbers in parentheses denote the percentage admixture of the one-quasiparticle state. The column labeled "Exact" gives the energies calculated by the shell-model method.

		Without term (5)		With term (5)	
J^π	Exact	Without g.s. correlation	With g.s. correlation	Without g.s. correlation	With g.s. correlation
$7/2^-$	0.0	0.0(98.1)	0.0(97.9)	0.0(98.4)	0.0(98.2)
$5/2^-$	0.84	1.12(0.12)	1.10(0.12)	1.14(0.13)	1.12(0.13)
$3/2^-$	1.39	1.72(0.05)	1.70(0.05)	1.74(0.06)	1.71(0.06)
$11/2^-$	1.91	2.13	2.10	2.15	2.12
$9/2^-$	2.10	2.30	2.27	2.32	2.30
$15/2^-$	2.79	3.06	3.03	3.07	3.04
$3/2_2^-$	3.76	3.34(94.0)	3.32(93.9)	3.68(94.6)	3.66(94.6)
$5/2_2^-$	5.16	4.93(67.0)	4.91(66.0)	5.22(69.1)	5.20(68.3)
$9/2_2^-$	5.36	5.15	5.12	5.45	5.43
$3/2_3^-$	5.37	5.01(2.60)	4.99(2.61)	5.31(2.37)	5.29(2.37)
$1/2^-$	5.50	5.09(34.2)	5.06(34.1)	5.43(33.2)	5.41(33.1)
$7/2_2^-$	5.67	5.30(0.02)	5.27(0.02)	5.62(0.02)	5.59(0.02)

Here $[a]$ stands for $2a+1$, N is the actual number of nucleons (protons in our case) present in the unfilled major shell, $\hat{\epsilon}_a$ is the single-particle shell-model energy corrected for self-energy, and $G(abcdJ)$ is the antisymmetric two-body matrix elements between angular-momentum-coupled states $\langle abJ|$ and $|cdJ\rangle$. The quasiparticle energy E_a, appearing in the above equations, is given by

$$E_a=[(\hat{\epsilon}_a-\lambda)^2+\Delta_a^2]^{1/2}. \tag{3}$$

The probability of occupancy V_a^2 and nonoccupancy U_a^2 of a given state a are determined from

$$U_a^2=\tfrac{1}{2}[1+(\hat{\epsilon}_a-\lambda)/E_a]$$

and

$$V_a^2=\tfrac{1}{2}[1-(\hat{\epsilon}_a-\lambda)E_a]. \tag{4}$$

The right-hand side of Eq. (2) is the expectation value of the number operator for the vacuum state of quasiparticles and applies to an even nucleus. For an odd-mass nucleus, the expectation value has to be taken for a single quasiparticle, say $|jm\rangle$. As a result, an extra term

$$(\hat{\epsilon}_j-\lambda)/E_j \tag{5}$$

has to be added to the right-hand side of the Eq. (2). Its effect is studied later.

The energy matrices to be diagonalized are

(a) With ground-state correlation

$$\begin{pmatrix} E & S & O & R \\ S & L+E' & -R & 0 \\ 0 & -R & -E & -S \\ R & 0 & -S & -L-E' \end{pmatrix} \tag{6}$$

and

(b) Without ground-state correlation

$$\begin{pmatrix} E & S \\ S & L+E' \end{pmatrix}, \tag{7}$$

respectively. Here E and E' are the unperturbed energies of one- and three-quasiparticle states, L is the matrix connecting three-quasiparticle subspaces, while S and R connect one- and three-quasiparticle and one- and three-quasihole subspaces, respectively. The explicit expressions for the matrices L, S, and R are contained in Ref. 11 through Eqs. (2.7)–(2.17).

TABLE III. Energy levels (MeV) of Mn^{53} by the MTDA method. All the levels are relative with respect to the lowest level. Numbers in parentheses denote the percentage admixture of the one-quasiparticle state. The results for MTDA with ground-state correlation differs little from MTDA without ground-state correlation (see Table II); hence they are not presented here.

J^π	$7/2^-$	$5/2^-$	$3/2^-$	$11/2^-$	$3/2_2^-$	$9/2^-$	$15/2^-$	$5/2_2^-$	$1/2^-$	$3/2_3^-$	$9/2_2^-$	$7/2_2^-$
Without term (5)	0.00	1.39	2.01	2.38	2.50	2.54	3.32	4.20	4.34	4.51	4.73	4.75
	(96.7)	(0.03)	(0.20)		(91.8)			(79.5)	(45.2)	(2.75)		(0.03)
With term (5)	0.00	1.48	2.09	2.45	2.83	2.61	3.38	4.54	4.71	4.89	5.17	5.15
	(97.1)	(0.03)	(0.01)		(92.5)			(81.8)	(46.6)	(2.54)		(0.02)

TABLE IV. Energy levels (MeV) of Co^{55} by the MTDA method. For other details see caption of Table III.

J^π	$7/2^-$	$3/2^-$	$5/2^-$	$3/2_2^-$	$5/2_2^-$	$11/2^-$	$9/2^-$	$1/2^-$	$3/2_3^-$	$15/2^-$	$7/2_2^-$
Without term (5)	0.00	1.25	2.26	2.83	3.03	3.23	3.37	3.40	4.04	4.15	4.22
	(95.3)	(91.2)	(0.49)	(0.64)	(89.6)			(70.0)	(1.41)		(0.03)
With term (5)	0.00	1.26	3.12	4.08	3.56	4.48	4.60	3.66	5.06	5.33	5.19
	(97.2)	(94.3)	(93.5)	(0.08)	(1.48)			(89.4)	(0.43)		(0.63)

2. NUMERICAL CALCULATION AND RESULTS

For the construction of energy matrices, one requires the two-body antisymmetric reaction matrix elements $G(abcdJ)$, which are tabulated in Ref. 5. With the help of these matrix elements, the hole-particle matrix elements $F(abcdJ)$ [Eq. (2.12) of Ref. 9] can be calculated which enter into the calculation. For the explicit numerical calculation of the levels of V^{51}, Mn^{53}, and Co^{55}, Ca^{48} was taken as an inert core and the protons in excess are assumed to be distributed in all possible ways among the $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ orbitals, the unperturbed single-particle energies for which were taken from Ref. 5 to be 0.0, 5.9, 4.4, and 6.9 MeV, respectively. The low-lying nuclear states of above nuclei are explained in terms of these four orbitals.

The parameters λ and Δ_a are obtained by solving the set of energy gap [Eq. (1)] and the number [Eq. (2)] with and without the extra term [Eq. (5)] by directly feeding the single-particle energies ϵ_a and the set of two-body pairing matrix elements $G(aabbo)$. These quantities in turn determine the quasiparticle energies E_a, given by Eq. (3) and the occupation (nonoccupation) probability $V_a^2(U_a^2)$ through Eq. (4) which comprise the second type of basic input data. The values of E and V with and without this extra term for V^{51}, Mn^{53}, and Co^{55} are tabulated in Table I.

The effect of the spurious 0^+ pair states from the three-quasiparticle basis states are eliminated by constructing their orthonormal set which are orthogonal to the spurious states, by the prescription given in Ref. 11, before the diagonalization of the energy matrices [Eqs. (6) and (7)].

The various matrices for spins and parity from $\frac{1}{2}^-$ to $\frac{15}{2}^-$ were generated, using the expressions (2.7)–(2.17) of Ref. 11 and diagonalized. The dimension of the matrices in the space of one- and three-quasiparticles for $\frac{1}{2}^-$, $\frac{3}{2}^-$, $\frac{5}{2}^-$, $\frac{7}{2}^-$, $\frac{11}{2}^-$, $\frac{13}{2}^-$, and $\frac{15}{2}^-$ were 12×12, 25×25, 28×28, 27×27, 23×23, 16×16, 8×8, and 5×5, respectively. The calculated energy levels for V^{51}, Mn^{53}, and Co^{55} are shown in the Table II–IV. Eigenvalues up to second $\frac{7}{2}^-$ are included and the percentage of one-quasiparticle component of the corresponding eigenvector is given in parentheses. In Table II, the second column corresponds to the energy values calculated by the shell-model method using the reaction matrix elements of Ref. 5.

Figure 1 shows a comparison of the experimental and calculated level spectra for V^{51}, Mn^{53}, and Co^{55}. Only the calculated levels obtained without the extra term [Eq. (5)] are included.

3. DISCUSSION AND CONCLUSIONS

From Table I, one can see that the inclusion of the extra term (5) in the BCS equations, causes a maximum change of 6 and 20% in E and V, respectively, for V^{51}, 8 and 10% for Mn^{53}, and 25 and 7% for Co^{55}. In the former two cases, these variations correspond to the single-particle state $\frac{3}{2}$, while in the last case it corresponds to the state $\frac{7}{2}$. The effect of mixing the one- and three-quasiparticle states is to slightly lower the energies of all the single-quasiparticle states; this lowering is appreciable in the case of single-quasiparticle states corresponding to $\frac{1}{2}^-$. This may be because of the fact that they contain relatively a large admixture of three-quasiparticle state (see Tables II–IV). The effect of including the correlation in the ground state (values are given only for V^{51}) changes the energy only slightly.

The results presented in Table II show that as far as the energy values and the components of the one-quasiparticle state are concerned, the descriptions of the first few states, with and without the extra term (5) and with and without ground-state correlation, are more or less the same. There is good agreement between the shell-model results (column two) and the MTDA results. The number of particles in the unfilled levels considered in this case is only three, the quasiparticle method is not expected to yield very good quantitative results for this nucleus, and therefore such an agreement should be taken as an indication about the reliability of the approximations involved in the quasiparticle method. The effect of the inclusion of the extra term (5) in the higher states gives rise to only a small change (although large compared to the changes in the lower states) in the energy which is mostly, in the right direction when compared with the values in column two, leaving the admixture of one-quasiparticle component practically unchanged. On the whole, the results with ground-state correlation are more or less very close to the one in which the extra term (5) is included or not. A similar trend is expected in the other cases and therefore only the MTDA results with the effect of the extra term (5) are presented for Mn^{53} and Co^{55}. The first five states

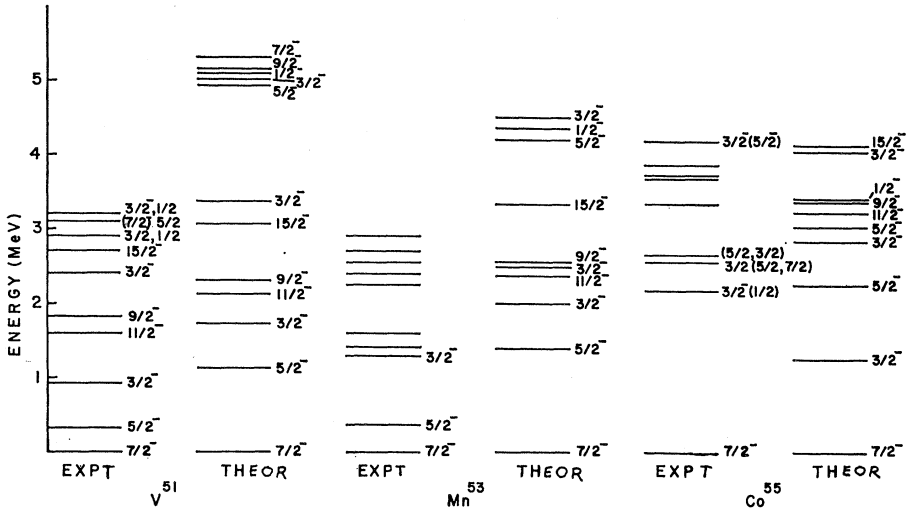

FIG. 1. Experimental (Expt) and theoretical (Theor) spectra of V^{51}, Mn^{53}, and Co^{55}.

(Table II) confirm the experimental ordering,[13] although their energies are relatively high. Except for the energy of the first $\frac{5}{2}^-$, the energies and ordering of the first six states are very close to the shell-model results calculated by assuming $(0f_{7/2})^3$ configuration for the protons as reported in Ref. 8. The ground state is predominantly of the one-quasiparticle type, while the first $\frac{5}{2}^-$ and $\frac{3}{2}^-$ states are practically a three-quasiparticle type. This is purely the effect of configuration mixing, due to which these three-quasiparticle states are pushed much lower than their predominantly one-quasiparticle states, which lie quite high.

Table III again reflects the fact that the effect of the extra term (5) on the energy values is quite small for the first few states but slightly greater than that in V^{51}, and causes comparatively a larger change in the energies of the higher states but the component of one-quasiparticle state in both the cases remains practically unchanged. In this case, as in V^{51}, the ground state is predominantly of the one-quasiparticle type and the first $\frac{5}{2}^-$ and $\frac{3}{2}^-$ are purely three-quasiparticle type and are pushed lower than their predominantly one-quasiparticle states as the result of configuration mixing. The experimental ordering[14] of the first two low-lying states is reproduced, but their energies are high. Except for the energy of the first $\frac{5}{2}^-$, and the second $\frac{3}{2}^-$ which is pushed below $\frac{1}{2}^{5}-$, the ordering and energies up to $\frac{1}{2}^{5}-$ are in reasonable agreement with the shell-model results calculated by assuming $(0f_{7/2})^{-3}$ configuration for the protons as reported in Ref. 8. The quality of agreement with and without the extra term (5) in the case of V^{51} and Mn^{53} is more or less the same.

The effect of the extra term (5) is more pronounced in the case of Co^{55} (Table IV). It causes reshuffling of some of the levels and even changes the component of the one-quasiparticle state. The ground state and the first $\frac{3}{2}^-$ remain predominantly of the one-quasiparticle type, while the predominance of the one-quasiparticle interchanges in the case of first and second $\frac{5}{2}^-$. The ordering of the first two excited states is consistent with the calculation of Kisslinger and Sorensen,[15] but no other theoretical results are known. Experimentally,[16] quite a large number of levels are known, but without knowing their definite spin and parity no comments can be made. On the basis of the results of Refs. 17 and 18, the spin and parity of the first excited state is consistent with the present result and there also appears a $\frac{3}{2}^-$ state around 4.175 MeV.

In general, the calculated energies are high compared with the observed ones (see Fig. 1). Experimentally, the energy of the first excited state in V^{51} and Mn^{53} is quite low (0.320 MeV in V^{51} and 0.376 MeV in Mn^{53}), but in Co^{55} it is comparatively too high ($\simeq$2.17 MeV). Since the quasiparticle theory describes the average property of the neighboring nuclei, it seems unlikely to explain such a change. Nevertheless, the MTDA method employing the reaction matrix elements of Kuo and Brown does describe the qualitative features of these nuclei.

ACKNOWLEDGMENTS

One of the authors (MLR) is grateful to the Research Foundation of the State University of New York for the financial support that he received during the course of this investigation. Thanks are also due to the staff of the Computing Center at the State University of New York at Buffalo, which is partially supported by NIH Grant No. FR-00126 and NSF Grant No. GP-7318 for providing the machine time.

[13] J. H. Towle, Nucl. Phys. **117**, 657 (1968).
[14] S. Sterner, L. Jonsson, and S. E. Arnell, Arkiv Fysik **31**, 567 (1965).
[15] L. S. Kisslinger and R. A. Sorensen, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **32**, No. 9 (1960).
[16] B. Erlandsson, Arkiv Fysik **34**, 263 (1967).
[17] D. S. Gemmell, L. L. Le, Jr., J. P. Schiffer, and A. B. Smith, Argonne National Laboratory Report No. ANL-6848, 1964 (unpublished).
[18] D. D. Armstrong and A. G. Blair, Phys. Rev. **140**, B1226 (1965).