ROTATIONS AND VIBRATIONS OF TWO AND THREE PARTICLES

THE QUANTUM THEORY OF THE ROTATIONS AND VIBRATIONS OF SIMPLE TWO- AND THREE-PARTICLE SYSTEMS

By

E. L. McFARLAND

A Thesis
Submitted to the School of Graduate Studies
in Partial Fulfilment of the Requirements
for the Degree
Master of Science

McMaster University
June 1970

MASTER OF SCIENCE (1970)
(Physics)

McMASTER UNIVERSITY
Hamilton, Ontario.

TITLE: The Quantum Theory of the Rotations and Vibrations of Simple Two- and Three-Particle Systems

AUTHOR: E. L. McFarland

SUPERVISOR: Professor A. B. Volkov

NUMBER OF PAGES: viii, 63

SCOPE AND CONTENTS:

This thesis examines the rotation-vibration spectra of systems of two and three particles (spin zero). The results in the two-particle case agree with many of the gross features of the spectra of deformed axially symmetric even-even nuclei. In the three-particle case, the set of basis functions used in the expansions of the wavefunctions was too small to give accurate eigenvalues and eigenvectors, but nevertheless the spectrum clearly corresponds to that of an asymmetric even-even nucleus.

ACKNOWLEDGEMENTS

It is a pleasure to thank Professor A. B. Volkov for his guidance, encouragement and constructive criticism throughout the period of this study. Thanks also must go to my fiancée Rosemary who spent many rather boring weekends with me while results for this thesis were being computed, and while the thesis itself was being written. I am also grateful to my office-mates for useful discussions pertaining to this work, and to the National Research Council of Canada for financial support. To Miss Cathy Wivell, I express my sincere appreciation for the typing and proofreading of this thesis.

PREFACE

The spectra of diatomic molecules have been studied for a long time(13); it is well known that such molecules have energy levels associated with rotational and vibrational motion, the energies of vibration being larger by a factor of about 1000 than those of rotation. One thus observes a band of rotational levels associated with a given vibrational state, i.e. the molecule is vibrating and rotating at the same time. Since the energies of the two modes of motion are well-separated, this means that the molecule vibrates about 1000 times during a single rotation, and hence the rotations and vibrations may be considered independent in a first approximation (Born-Oppenheimer or Adiabatic Approximation(19,20)). If one assumes that the molecule is a rigid rotor, then the energies in a given rotational band follow a simple J(J+1) dependence, where J is the angular momentum. This J(J+1) dependence is experimentally observed, but the dependence is not quite exact; however, the discrepancies can be accounted for by including stretching effects as the angular momentum increases.

In nuclei as well, energy levels are found which are associated with rotational and vibrational motion. In even-even axially symmetric nuclei, rotational bands of even J and positive parity are often found, with an approximate

J(J+1) energy dependence. Such a band may be built on the ground state ($J\pi = 0+$), or on an excited 0+ state which has the characteristics of a so-called β-vibration, i.e. a vibration which maintains the axial symmetry. (It is also possible to have a so-called γ-band, a rotational band built on a γ-vibration [axial symmetry not maintained] - the level ordering in this case is 2+, 3+, 4+, ...) It seems quite astounding, at first sight, that in the nuclear case, in which the energies (and hence rates of motion) of vibrations and rotations are of comparable magnitude, one gets results similar to the molecular case. There are several interesting features in these nuclear rotational bands, in addition to this approximate J(J+1) energy dependence. The reduced transition matrix elements (the B(E2)'s) for electric quadrupole transitions between states in the same band are much greater than those for transitions between states in different bands. Also, if a state of high J in a band other than the ground state band (g.s.b.) is excited, favourable energy differences lead to cross-band transitions towards the g.s.b. with little loss of angular momentum(14), and thus it is difficult to observe levels of low J in the excited rotational band. The set of lowest observed levels in the various bands, i.e. those levels which can be populated with reasonable probability before cross-band transitions (towards the g.s.b.) depopulate the band, usually have lower J values for the lower vibrational bands. The locus of these levels can be used to define the so-called "Yrast" line$^{(15)}$ which is composed of the "Yrast" levels. The above feature can be summarized by saying that the system tends to decay via the Yrast levels. This thesis reproduces these qualitative features of such nuclear rotational - vibrational bands from a simple model in which an axially symmetric nucleus is represented by two spinless particles interacting via a potential.

Nuclear states are also observed which indicate rotational bands resulting from rotations of an asymmetric nucleus, or alternatively from rotations of a nucleus which is axially symmetric in its ground state, but has been excited by a γ-vibration (a vibration which does not preserve axial symmetry) to an asymmetric shape. In a band of this type, there are found to be $\frac{J}{2} + 1$ states of a given J for J even, and $\frac{J-1}{2}$ states of a given J for J odd. This corresponds exactly with the number of states for a given J that results from assuming a rigid asymmetric rotor with wavefunctions that transform according to the A-representation (totally symmetric) of the D_2 group$^{(17,18)}$ (Appendix C). For a completely rigid object, it is also found that the sum of the energies of the states of a given even J equals the sum of the energies of the states of angular momentum (J+1). This relation is satisfied approximately (within 1 or 2%) by several nuclei. As well, in observed rotational bands of this type, the B(E2)'s for in-band transitions

are larger than those for extra-band transitions. This thesis investigates the rotational-vobrational spectrum of a simple asymmetric system consisting of three spinless particles, and finds that although the calculation was not accurate enough to give good eigenvalues and eigenvectors, the results indicate the presence of rotational bands of the above type, with the B(E2)'s for in-band transitions greater than those for extra-band transitions.

TABLE OF CONTENTS

CHAPTER I

THEORY: TWO-PARTICLE PROBLEM

Introduction

The problem of two identical particles (spin zero) of mass m may be considered in terms of the equivalent one-particle problem, the Schrodinger equation of which is:

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(r,\theta,\phi) + V(r)\,\psi(r,\theta,\phi) = E\,\psi(r,\theta,\phi) \qquad (1)$$

where $\mu = \frac{m}{2}$ is the reduced mass, $\underline{r}$ represents the relative co-ordinates of the two particles, and V(r) is a central potential. In the discussion which follows, V(r) is taken to be the sum of an attractive and a repulsive Gaussian:

$$V(r) = V_a\, e^{-K_a r^2} + V_r\, e^{-K_r r^2} \qquad .(2)$$

By variation of the parameters V_a, V_r, K_a and K_r, a wide range of potentials may be generated.

In order to solve Eq. (1) for eigenvalues and eigenvectors, ψ is approximated by a linear combination of a complete set of functions:

$$\psi_{NJM} = Y_J^M(\theta,\phi) \sum_n c_n\, \phi_{nJ}(r) \qquad (3)$$

where N is used to distinguish the many wavefunctions which have a given J and M. The Y_J^M are the usual spherical harmonics:

$$Y_J^M(\theta,\phi) = \sqrt{\frac{(2J+1)}{4\pi}\,\frac{(J-M)!}{(J+M)!}}\; P_J^M(\cos\,\theta)\; e^{iM\phi} \tag{4}$$

$$\int Y^{*M'}_{J'}(\theta,\phi)\; Y_J^M(\theta,\phi)\,d\Omega = \delta_{JJ'}\;\delta_{MM'} \quad . \tag{5}$$

The label J is used here instead of the customary L, since in this problem the particles are spinless and the total angular momentum J equals the orbital angular momentum L. The $\phi_{nJ}(r)$ (1) are the radial parts of the solution of the three-dimensional spherical harmonic oscillator problem:

$$\phi_{nJ}(r) = \left[\frac{2n!}{\Gamma(n+J+\frac{3}{2})}\right]^{\frac{1}{2}} (\beta r^2)^{\frac{J}{2}}\; e^{-\frac{1}{2}\beta r^2}\; L_n^{J+\frac{1}{2}}(\beta r^2) \tag{6}$$

where $\beta = \frac{\mu\omega}{\hbar}$, ω being the oscillator frequency, and $L_n^{J+\frac{1}{2}}$ is a Laguerre Polynomial as defined in Erdelyi et. al.(2):

$$L_n^{\alpha}(x) = \sum_{s=0}^{n} \frac{(n+\alpha)!\;\;(-x)^s}{(n-s)!\;\;(\alpha+s)!} \quad . \tag{7}$$

The expansion in Eq. (3) is merely an approximation since the summation cannot run over the infinite number of values of n. However, the maximum value of n is chosen large enough so as to give a good approximation to the true ψ. The "goodness of approximation" is measured by the values of the c_n. As n increases, $|c_n|$ tends to decrease until it is effectively zero; at this point, the set of basis functions ϕ_{nJ} may be truncated with little loss of accuracy in either ψ or E. Since the basis is truncated, the eigenvalues and eigenvectors are dependent on the value of β which is chosen. The criterion for determining the optimum value of β is the minimization of the ground state energy of the system (Variational Principle).

It is convenient to define a dimensionless parameter r':

$$r' = \sqrt{\beta}\, r = \frac{r}{b} \qquad ,(8)$$

where $b = \frac{1}{\sqrt{\beta}}$ has dimensions of length. Then the ϕ_{nJ} may be written:

$$\phi_{nJ}(r') = \left[\frac{2n!}{\Gamma(n+J+\frac{3}{2})}\right]^{\frac{1}{2}} r'^{J}\, e^{-\frac{1}{2}r'^2}\, L_n^{J+\frac{1}{2}}(r'^2) \qquad (9)$$

The ϕ_{nJ}'s are normalized:

$$\int \phi^*_{n'J}(r')\, \phi_{nJ}(r')\, r'^2 dr' = \delta_{n'n} \qquad .(10)$$

Substitution of $r' = \frac{r}{b}$ in Eq. (1) gives:

$$\left[-\frac{\hbar^2}{2\mu}\frac{\nabla^2_{r'}}{b^2} + V(r')\right]\psi = E\,\psi \qquad (11)$$

where
$$V(r') = V_a\, e^{-K_a b^2 r'^2} + V_r\, e^{-K_r b^2 r'^2} \qquad (12)$$

and $\nabla^2_{r'}$ is the Laplacian operator in the (r',θ,ϕ) system. If all energies are now expressed in units of μc^2, and all lengths in units of $\frac{\hbar}{\mu c}$, Eq. (11) becomes:

$$[-\frac{1}{2b^2}\nabla^2_{r'} + V'(r')]\psi = E'\ \psi \tag{13}$$

where $$V'(r') = \frac{V(r')}{\mu c^2}, \quad \text{and} \quad E' = \frac{E}{\mu c^2} \quad .$$

With ψ as in Eq. (3), the problem now consists of constructing the matrix elements

$$H_{\substack{nJM\\n'J'M'}} = \langle\phi_{nJ}(r')Y_J^M(\theta,\phi)|-\frac{1}{2b^2}\nabla^2_{r'}+V'(r')|\phi_{n'J'}(r')Y_{J'}^{M'}(\theta,\phi)\rangle$$

and diagonalizing the ensuing matrix.

Evaluation of Matrix Elements

Using

$$\langle\phi_{nJ}(r')Y_J^M(\theta,\phi)|-\tfrac{1}{2}\nabla^2_{r'}+\tfrac{1}{2}r'^2|\phi_{n'J'}(r')Y_{J'}^{M'}(\theta,\phi)\rangle = \delta_{nn'}\delta_{JJ'}\delta_{MM'} \times (2n+J+\tfrac{3}{2}),$$

then

$$H_{\substack{nJM\\n'J'M'}} = \delta_{JJ'}\delta_{MM'}\{\frac{1}{b^2}[\delta_{nn'}(2n+J+\tfrac{3}{2})-\tfrac{1}{2}\langle\phi_{nJ}(r')|r'^2|\phi_{n'J'}(r')\rangle] + \langle\phi_{nJ}(r')|V'(r')|\phi_{n'J'}(r')\rangle\} \quad . \tag{14}$$

Clearly the simplest procedure to follow is to construct matrices in subspaces of given J and diagonalize these submatrices individually, since the Hamiltonian does not mix states of different J. The above matrix elements are independent of M, so that each eigenvalue of given J will be (2J+1)-fold degenerate. This is to be expected, since the Hamiltonian is rotationally invariant. The matrix element of expression (14) will hence be labelled as $H_{nn'}^{J}$.

To evaluate the matrix elements $\langle\phi_{nJ}(r')|r'^2|\phi_{n'J'}(r')\rangle$, use is made of a recursion relation for the Laguerre polynomial$^{(2)}$:

$$r'^2\, L_n^{\alpha}(r'^2) = -(n+1)\, L_{n+1}^{\alpha}(r'^2) - (n+\alpha)\, L_{n-1}^{\alpha}(r'^2) + (2n+\alpha+1) \times L_n^{\alpha}(r'^2) \qquad .(15)$$

Hence

$$r'^2\, \phi_{nJ}(r') = -\sqrt{(n+1)(n+J+\tfrac{3}{2})}\, \phi_{n+1,J}(r') - \sqrt{n(n+J+\tfrac{1}{2})} \times \phi_{n-1,J}(r') + (2n+J+\tfrac{3}{2})\, \phi_{nJ}(r') \qquad .(16)$$

Then using Eq. (10), the result is:

$$\langle\phi_{nJ}(r')|r'^2|\phi_{n'J}(r')\rangle = -\sqrt{(n+1)(n+J+\tfrac{3}{2})}\, \delta_{n',n+1} - \sqrt{n(n+J+\tfrac{1}{2})}\, \delta_{n',n-1} + (2n+J+\tfrac{3}{2})\, \delta_{n',n} \qquad .(17)$$

The matrix elements $\langle\phi_{nJ}(r')|V'(r')|\phi_{n'J'}(r')\rangle$ are evaluated as follows. Consider a typical matrix element of the form:

$$<\phi_{nJ}(r')|e^{-\gamma r'^2}|\phi_{n'J}(r')> = N_{n'J}N_{nJ}\int_0^\infty e^{-(\gamma+1)r'^2} r'^{2J}$$

$$\times L_n^{J+\frac{1}{2}}(r'^2)\ L_{n'}^{J+\frac{1}{2}}(r'^2)\ r'^2 dr',$$

where $N_{nJ} = [\frac{2n!}{\Gamma(n+J+\frac{3}{2})}]^{\frac{1}{2}}$. Substitution of $\chi = r'^2$ gives

$$\frac{N_{n'J}N_{nJ}}{2}\int_0^\infty e^{-(\gamma+1)\chi}\ \chi^{J+\frac{1}{2}}\ L_n^{J+\frac{1}{2}}(\chi)\ L_{n'}^{J+\frac{1}{2}}(\chi)\,d\chi = \frac{N_{n'J}N_{nJ}}{2}\ \frac{\Gamma(n'+n+J+\frac{3}{2})}{n'!\ n!}$$

$$\times \frac{\gamma^{n'+n}}{(\gamma+1)^{n'+n+J+\frac{3}{2}}}$$

$$\times\ {}_2F_1[-n',-n;-n'-n-J-\tfrac{1}{2}\ ;\ \frac{(\gamma+1)(\gamma-1)}{\gamma^2}] \qquad (18)$$

from Erdelyi et. al.$^{(4)}$, where ${}_2F_1$ is a generalized hypergeometric function defined by$^{(5)}$:

$${}_mF_n(a_1,\ldots,a_m;\gamma_1,\ldots,\gamma_n;z) = \sum_{k=0}^{\infty} \frac{(a_1)_k\ldots(a_m)_k}{(\gamma_1)_k\ldots(\gamma_n)_k}\,\frac{z^k}{k!} \quad .$$

The symbol $(\lambda)_k$ denotes the quantity

$$(\lambda)_k = \frac{\Gamma(\lambda+k)}{\Gamma(\lambda)}\ ,\ k = 1,2,\ldots\quad ;\quad (\lambda)_0 = 1 \quad .$$

Using Eqs. (17) and (18) all matrix elements $H_{\substack{nn'\\J}}$ can be easily calculated. The matrix may then be diagonalized and eigenvalues and eigenvectors obtained.

It should be noted here that we shall consider only states of even J and positive parity are in this problem. The parity operation corresponds to an interchange of the particles; and if we assume that the particles are identical bosons, then the wavefunction must not change sign under particle interchange, and hence the wavefunction must have positive parity, i.e. $(-)^J = +$, and thus J must be even. This symmetry requirement is similar to that for axially symmetric, deformed even-even nuclei.

Electric Quadrupole Transitions

It is interesting to examine the electric quadrupole transition probabilities for transitions between the eigenstates. The transition probability for an electric quadrupole photon of energy $\hbar\omega = \hbar ck$, of z-projection u, with the nucleus going from a state i to a state f is (6):

$$T_{if}(E2u) = \frac{12\pi}{225}\frac{k^5}{\hbar} \left|\langle f|Q_{2u}|i\rangle\right|^2 \tag{19}$$

where Q_{2u} is the electric quadrupole operator:

$$Q_{2u} = \sum_i e_i\, r_i^2\, Y_2^{*u}(\theta_i,\phi_i) \quad . \tag{20}$$

The sum is over charged particles; in the problem at hand, there is effectively only one particle, the effective charge

e_{eff} of which must be determined. To do this, we consider the two actual charges as point charges. Then the electric quadrupole moment is:

$$e_1 r_1^2 + e_2 r_2^2 = 2er_1^2 \quad ,$$

since $e_1=e_2=e$ and $|\underline{r}_1| = |\underline{r}_2|$. In the equivalent one-particle problem, the electric quadrupole moment is:

$$e_{eff}\ r^2 = 4\ e_{eff}\ r_1^2 \quad ,$$

since $|\underline{r}| = 2|\underline{r}_1|$. Hence $4\ e_{eff} = 2e$, and $e_{eff} = \frac{e}{2}$, that is, the effective charge is equal to one-half of the charge on each of the actual particles.

Since the orientation of the nucleus is of little interest, the expression (19) is summed over M_f and M_i (the z-projections of the angular momenta in states f and i, respectively) and averaged over M_i to give:

$$T(E2) = \frac{12\pi}{225}\frac{k^5}{\hbar}\ B(E2) \qquad (21)$$

where B(E2) is the so-called reduced matrix element:

$$B(E2,J_i \rightarrow J_f) = \frac{1}{(2J_i+1)} \sum_{M_i,M_f} |\langle f|Q_{2u}|i\rangle|^2 \quad .(22)$$

Only one value of u, that is, $u = M_f - M_i$ contributes to each term in the sum. Clearly, if $|M_f - M_i| > 2$, then the matrix element $<f|Q_{2u}|i>$ is zero. To calculate the non-zero values of $<f|Q_{2u}|i>$, the Wigner-Eckart theorem(7) is used:

$$<N_fJ_fM_f|Q_{2u}|N_iJ_iM_i> = <N_fJ_f||Q_2||N_iJ_i> <J_i2M_iu|J_fM_f> \quad .(23)$$

The symbol $<N_fJ_f||Q_2||N_iJ_i>$, which is independent of the M's, is also called the reduced matrix element; to avoid confusion, this will be referred to as the RME. The simplest procedure to follow now is to calculate $<N_fJ_fM_f|Q_{2u}|N_iJ_iM_i>$ for say, $M_f = M_i = u = 0$. Then the RME is:

$$<N_fJ_f||Q_2||N_iJ_i> = \frac{<N_fJ_f0|Q_{20}|N_iJ_i0>}{<J_i200|J_f0>} \quad .(24)$$

Using the value for the RME obtained from (24), it is then easy to calculate any $<N_fJ_fM_f|Q_{2u}|N_iJ_iM_i>$ as the product of the RME and the appropriate Clebsch-Gordon coefficient. The value for B(E2) may then be obtained from (22), and the transition probability T(E2) from (21).

Thus, the problem now is reduced to the calculation of the matrix element:

$$<N_fJ_f0|Q_{20}|N_iJ_i0>$$

$$= <\psi_{N_fJ_f0}\left|\frac{e}{2} r^2 Y_2^0(\theta,\phi)\right|\psi_{N_iJ_i0}>$$

$$= \frac{e}{2\beta}\int Y^{*0}_{J_f}(\Omega)\, Y_2^0(\Omega)\, Y^0_{J_i}(\Omega)d\Omega \int (\sum_{n_f} c_{n_f}\, \phi_{n_fJ_f}(r'))r'^2$$

$$\times (\sum_{n_i} c_{n_i}\, \phi_{n_iJ_i}(r'))r'^2 dr' \quad .(25)$$

The angular integral is found in Rose$^{(8)}$:

$$\int Y_{J_f}^{*0}\, Y_2^0\, Y_{J_i}^0 \, d\Omega = \left[\frac{5}{4\pi}\,\frac{(2J_i+1)}{(2J_f+1)}\right]^{\frac{1}{2}} (\langle J_i 0\ 20 | J_f 0\rangle)^2 \qquad .(26)$$

Write the radial integral as:

$$\sum_{n_f} \sum_{n_i} c_{n_f}\, c_{n_i}\, I_{n_f,J_f,n_i,J_i}$$

where

$$I_{n_f,J_f,n_i,J_i} = \langle \phi_{n_f J_f} | r'^2 | \phi_{n_i J_i} \rangle \qquad .$$

For $J_f=J_i=J$, I is given by Eq. (17) and the radial integral is:

$$\sum_{n_f} \sum_{n_i} c_{n_f}\, c_{n_i} \Big(-\sqrt{(n_i+1)(n_i+J+\tfrac{3}{2})}\ \delta_{n_f,n_i+1} - \sqrt{n_i(n_i+J+\tfrac{1}{2})}\ \delta_{n_f,n_i-1}$$

$$+ (2n_i+J+\tfrac{3}{2})\ \delta_{n_f,n_i}\Big) \qquad .(27)$$

For J_f and J_i differing by 2,

$$I = \int_0^\infty N_{n_f,J+2}\, r'^{J+2}\, e^{-\frac{1}{2}r'^2}\, L_{n_f}^{J+\frac{5}{2}}(r'^2)\, r'^2\, N_{n_i,J}\, r'^J\, e^{-\frac{1}{2}r'^2}$$

$$\times\ L_{n_i}^{J+\frac{1}{2}}(r'^2)\, r'^2 dr' \qquad ,(28)$$

where it has been assumed that $J_f=J_i+2=J+2$. To evaluate expression (28), a recursion relation is used$^{(3)}$:

$$r'^2\, L_n^{\alpha+1}(r'^2) = (n+\alpha+1)\ L_n^{\alpha}(r'^2) - (n+1)\ L_{n+1}^{\alpha}(r'^2) \qquad .(29)$$

Using this relation twice to dispose of the r'^2 operator, and of the r'^2 in the r'^{J+2} term above,

$$r'^2 r'^2 L_{n_f}^{J+\frac{5}{2}}(r'^2) = (n_f+J+\tfrac{5}{2})(n_f+J+\tfrac{3}{2})\, L_{n_f}^{J+\frac{1}{2}}(r'^2) - 2(n_f+J+\tfrac{5}{2}) \times (n_f+1)\, L_{n_f+1}^{J+\frac{1}{2}}(r'^2) + (n_f+1)(n_f+2) \times L_{n_f+2}^{J+\frac{1}{2}}(r'^2) \quad .(30)$$

Hence,

$$r'^2\, \phi_{n_f,J+2}(r') = (n_f+J+\tfrac{5}{2})^{\frac{1}{2}}(n_f+J+\tfrac{3}{2})^{\frac{1}{2}}\, \phi_{n_f,J}(r') - 2(n_f+J+\tfrac{5}{2})^{\frac{1}{2}} \times (n_f+1)^{\frac{1}{2}}\, \phi_{n_f+1,J}(r') + (n_f+1)^{\frac{1}{2}}(n_f+2)^{\frac{1}{2}} \times \phi_{n_f+2,J}(r')$$

and

$$I = (n_f+J+\tfrac{5}{2})^{\frac{1}{2}}(n_f+J+\tfrac{3}{2})^{\frac{1}{2}}\, \delta_{n_f,n_i} - 2(n_f+J+\tfrac{5}{2})^{\frac{1}{2}}(n_f+1)^{\frac{1}{2}}\, \delta_{n_f+1,n_i} + (n_f+1)^{\frac{1}{2}}(n_f+2)^{\frac{1}{2}}\, \delta_{n_f+2,n_i} \quad .(31)$$

For the case of $J_i = J_f+2 = J+2$, the roles of initial and final states are simply reversed in the above derivation.

Thus, using I from (17) or (31), and the angular integral from (26), the matrix element (25) may be evaluated, and hence the B(E2) and the T(E2). The 2 cases of

$J_f = J_i$, and J_f and J_i differing by 2 need be considered only, since the quadrupole operator connects only states differing in J by 2 or less. Since symmetry assumptions eliminate odd J states, it is unnecessary to consider J_f and J_i differing by 1.

CHAPTER II

THEORY: THREE PARTICLE PROBLEM

The case of three particles is of course much more complicated than that of two particles. The Hamiltonian of the problem is:

$$H = \sum_{i=1}^{3} T_i + \sum_{i<j=1}^{3} V_{ij} - T_{CM} \qquad ,(1)$$

where T_i is the particle kinetic energy, T_{CM} is the kinetic energy associated with the centre of mass of the system, and V_{ij} is the same two-particle potential as in the two-particle problem of Chapter I. The potential energy is summed over all two-particle interactions.

Again, the wavefunction is approximated by a linear combination of a complete set of functions:

$$\psi(\underline{r}_1,\underline{r}_2,\underline{r}_3) = \sum_k C_k \, \psi_k(\underline{r}_1,\underline{r}_2,\underline{r}_3) \qquad .(2)$$

Of course, the sum must be truncated after a finite number of terms. The basis functions ψ_k which are used are properly symmetrized combinations of single particle basis functions, which are cylindrical harmonic oscillator wavefunctions:

$$\chi_{n,m,n_z}(\sqrt{\alpha}\,\rho,\phi,\sqrt{a}\,z) = P_{n,m}(\sqrt{\alpha}\,\rho)\,\Phi_m(\phi)\,Z_{n_z}(\sqrt{a}\,z) \qquad (3)$$

where $\alpha = \frac{m\omega_\rho}{\hbar}$, $a = \frac{m\omega_z}{\hbar}$, and ω_ρ and ω_z are the oscillator frequencies.

$$P_{n,m}(\sqrt{\alpha}\ \rho) = [\frac{2\ \alpha\ n!}{(n+|m|)!}]^{\frac{1}{2}}\ (\sqrt{\alpha}\ \rho)^{|m|}\ L_n^{|m|}(\alpha\rho^2)\ e^{-\frac{1}{2}\alpha\rho^2}$$

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}\ e^{im\phi}$$

$$Z_{n_z}(\sqrt{a}\ z) = [\frac{a^{\frac{1}{2}}}{\pi^{\frac{1}{2}}\ 2^{n_z}\ n_z!}]^{\frac{1}{2}}\ H_{n_z}(\sqrt{a}\ z)\ e^{-\frac{1}{2}az^2} \quad .(4)$$

The wavefunctions (3) are eigenfunctions of

$$[-\frac{\hbar^2}{2m}\nabla^2 + \frac{m\omega_\rho^{\ 2}}{2}\rho^2 + \frac{m\omega_z^{\ 2}}{2} z^2]\ \chi_{n,m,n_z} = E_{n,m,n_z}\ \chi_{n,m,n_z}$$

with $$E_{nmn_z} = (2n+|m|+1)\hbar\omega_\rho + (n_z+\tfrac{1}{2})\hbar\omega_z \quad .$$

In the calculations which follow, $\omega_\rho = \omega_z = \omega$ and hence α=a; thus, a spherical harmonic oscillator representation could have been used, but the cylindrical representation was chosen to facilitate calculation of the potential matrix elements. Since the set of basis functions ψ_k is truncated, the eigenvalues and eigenvectors depend on the value of α(a). The value of α which gives the minimum ground state energy is chosen, just as in the two-particle problem.

If the set of quantum numbers n,m,n_z is represented by q, then the symmetrized three-body wavefunction ψ_k can be written:

$$\psi_k = \frac{1}{\sqrt{A}} \sum_p P \prod_{i=1}^{3} \chi_{q_i}(\underline{r}_i) \qquad (5)$$

where P is a permutation operator which permutes the coordinates $\underline{r}_i$, and the sum is over all such possible permutations. If all the q_i are different, there are 6 possible permutations, and hence the normalization factor is $\frac{1}{\sqrt{A}} = \frac{1}{\sqrt{6}}$; similarly, if all the q_i are the same, $\frac{1}{\sqrt{A}} = 1$, and if only 2 of the q_i are the same, $\frac{1}{\sqrt{A}} = \frac{1}{\sqrt{3}}$.

The problem is now to construct matrix elements of the Hamiltonian (1) between wavefunctions of the form (5), and then to diagonalize the matrix. Since the Hamiltonian is rotationally invariant, it is possible to diagonalize separately submatrices constructed from matrix elements of H between states of definite J and M; as well, for a given J, the matrix elements will be independent of M, and hence each eigenstate of angular momentum J will be (2J+1)-fold degenerate. However, since it is non-trivial to construct states of definite J (the wavefunctions χ are not eigenfunctions of angular momentum), only states of definite M will be constructed. Diagonalization then proceeds in each M-subspace (for all $M>0$), and the J-value of each resulting eigenvalue is equal to the largest M-value for which this eigenvalue exists. It is easy to construct three-particle basis states ψ_k of definite M, since all that is required is that $\sum_{i=1}^{3} m_i = M$ (6), where the m_i refer to the m-values of the

3 single-particle states. We also require that the basis states ψ_k be of positive parity. Since the parity π_i of a wavefunction χ_{q_i} is $(-1)^{(2n_i+|m_i|+n_{z_i})}$, this means that $\prod_{i=1}^{3} \pi_i = +1$.

Although the kinetic energy of the centre of mass has been subtracted in the Hamiltonian (1), it is still possible to have eigenstates which have spurious centre of mass excitations. Clearly, these states are of no interest, and a method must be devised to identify which states include centre of mass excitations. The method adopted is to add a term of the form

$$\mathrm{FAC} \; . \; [\frac{P^2}{2M} + \tfrac{1}{2} M \omega^2 R^2]$$

(7) to the Hamiltonian, where the mass M = 3m (not to be confused with the quantum numbers M and m of Eq. (6)) is the total mass of the system, $\underline{P} = \sum_{i=1}^{3} \underline{p}_i$ is the centre of mass momentum, and $\underline{R} = \sum_{i=1}^{3} \underline{r}_i$ represents the centre of mass co-ordinates. FAC is a suitably chosen large number (∿ 5000 worked well). The reason for the addition of this term is that any spurious centre of mass excitations which do occur are eigenstates of an oscillator with frequency ω. The eigenvalues are therefore $(n + \frac{3}{2})\hbar\omega$, where n is a positive integer or zero. Thus the inclusion of the term (7) in the Hamiltonian, if FAC is chosen large enough, has the effect of separating all eigenstates into sets of states corresponding to the various centre of mass excitations (Fig. 1). The lowest set

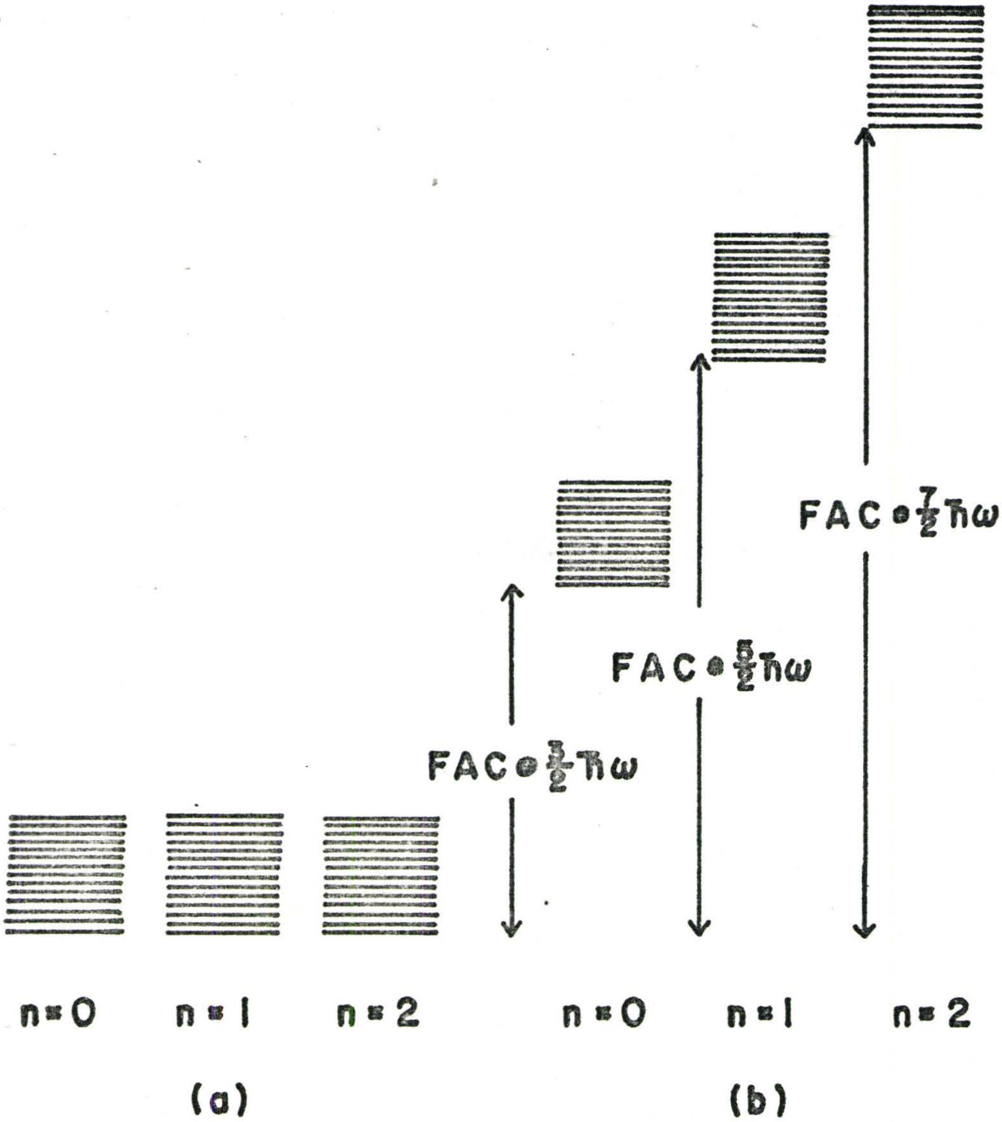


FIGURE 1

CENTRE OF MASS EXCITATIONS

(a) It is normally difficult to identify centre of mass excited states.

(b) Identification of centre of mass states is now trivial.

of states has no centre of mass excitation $(n=0)$; hence, each state will have an energy of FAC . $(\frac{3}{2}\hbar\omega)$ above the energy that would occur without the inclusion of term (7) in the Hamiltonian. The second set of states $(n=1)$ is raised by an energy of FAC . $(\frac{5}{2}\hbar\omega)$ above the energies that would result without term (7), and so on. Once the centre of mass excited states have been identified, the extra centre of mass contribution from (7) is subtracted from the eigenvalues. For a wavefunction ψ of the form (2), this centre of mass correction is:

$$- \sum_k \sum_\ell c_k c_\ell \langle\psi_k(\underline{r}_1,\underline{r}_2,\underline{r}_3)\,|\,\text{FAC} \,.\, (\frac{P^2}{2M} + \tfrac{1}{2}M\,\omega^2\,R^2)\,|\,\psi_\ell(\underline{r}_1,\underline{r}_2,\underline{r}_3)\rangle .$$

This procedure works only if the three-particle basis states ψ_k which are used consist of all possible combinations of 3 single particle basis states χ_q which represent a total "excitation energy" less than or equal to $N\hbar\omega$ above the basis ground state which consists of all three particles in the lowest oscillator state χ. N is a positive integer or zero. Since the excitation energy of a state χ_q is $(2n+|m|+n_z)\hbar\omega$, and since the requirement of positive parity means that $\prod_{i=1}^{3} (-1)^{(2n_i+ m_i +n_{z_i})} = +1$, hence N must be even. Thus, the above centre of mass method can be used with basis states ψ_k representing excitations of up to $2\hbar\omega$, $4\hbar\omega$, $6\hbar\omega$, etc. Clearly, each increase in excitation of $2\hbar\omega$ will give more basis states to work with, and thus the approximation to the wavefunction ψ will be better.

Matrix Elements

With the inclusion of term (7), the Hamiltonian now has the form:

$$H = \frac{\hbar^2}{2m} \sum_{i=1}^{3} k_i^2 + \sum_{i<j} V_{ij} - [\frac{\hbar^2}{6m} \sum_i k_i^2 + \frac{\hbar^2}{3m} \sum_{i<j} \underline{k}_i \cdot \underline{k}_j]$$

$$+ \text{FAC} \, . \, [\frac{\hbar^2}{6m} \sum_i k_i^2 + \frac{\hbar^2}{3m} \sum_{i<j} \underline{k}_i \cdot \underline{k}_j + \tfrac{1}{2} \frac{m\omega^2}{3} \sum_i r_i^2 + \frac{m\omega^2}{3} \sum_{i<j}$$

$$\times \, \underline{r}_i \cdot \underline{r}_j] \qquad (8)$$

where we have written $\underline{p}=\hbar\underline{k}$. If energy is expressed in units of mc^2, and length in units of $\frac{\hbar}{mc}$, H may be written:

$$H = \{(\frac{1}{3} + \frac{\text{FAC}}{6}) \sum_i k_i^2 + \frac{\alpha^2 \, \text{FAC}}{6} \sum_i r_i^2\}$$

$$+ \{\sum_{i<j} V'_{ij} + \frac{1}{3}(\text{FAC}-1) \sum_{i<j} \underline{k}_i \cdot \underline{k}_j + \frac{\alpha^2}{3} \text{FAC} \sum_{i<j}$$

$$\times \, \underline{r}_i \cdot \underline{r}_j\} \qquad (9)$$

where $V'_{ij} = \frac{V_{ij}}{mc^2}$, and the brackets {...} contain one-body and two-body operators respectively. Matrix elements of the following form are required:

$$H_{k\ell} = \langle\psi_k|H|\psi_\ell\rangle$$

$$= \int \left(\frac{1}{\sqrt{B}} \sum_{p'} P' \prod_{i=1}^{3} \chi_{q_i}(\underline{r}_i)\right)^* H\left(\frac{1}{\sqrt{A}} \sum_{p} P \prod_{i=1}^{3} \chi_{s_i}(\underline{r}_i)\right)$$

$$\times\ d\tau_1\ d\tau_2\ d\tau_3 \qquad .(10)$$

Consider a typical term in $H_{k\ell}$:

$$\int \left(\frac{1}{\sqrt{B}} P' \prod_{i=1}^{3} \chi_{q_i}(\underline{r}_i)\right)^* H\left(\frac{1}{\sqrt{A}} \sum_{p} P \prod_{i=1}^{3} \chi_{s_i}(\underline{r}_i)\right) d\tau_1\ d\tau_2\ d\tau_3 \qquad .(11)$$

Since the $\underline{r}_i$ are merely dummy variables, they can be relabelled in any desired manner and the term (11) becomes simply:

$$\int \left(\frac{1}{\sqrt{B}} \prod_{i=1}^{3} \chi_{q_i}(\underline{r}_i)\right)^* H\left(\frac{1}{\sqrt{A}} \sum_{p} P \prod_{i=1}^{3} \chi_{s_i}(\underline{r}_i)\right) d\tau_1\ d\tau_2\ d\tau_3\ .$$

This argument can be applied to each of the B P'-permutations, and hence $H_{k\ell}$ can be written:

$$H_{k\ell} = \sqrt{\frac{B}{A}} \sum_{p} \int \left(\prod_{i=1}^{3} \chi^*_{q_i}(\underline{r}_i)\right) (H_1+H_2) \left(P \prod_{i=1}^{3} \chi_{s_i}(\underline{r}_i)\right) d\tau_1\ d\tau_2\ d\tau_3 \qquad (12)$$

where H_1 and H_2 are the one-body and two-body parts of the Hamiltonian, respectively. If all the q_i are different from the s_i, then $H_{k\ell}$ is trivially zero. If one of the q_i is the same as one of the s_i, then we get a contribution to $H_{k\ell}$ from H_2; if two of the q_i's are the same as two of the s_i's, or if $H_{k\ell}$ is diagonal, there is a contribution to $H_{k\ell}$ from both H_1 and H_2. In these three cases, $H_{k\ell}$ reduces to sums of integrals of the forms:

$$\int \chi_q^*(\underline{r})\ r^2\ \chi_s(\underline{r})\ d\tau = \langle q|r^2|s\rangle$$

$$\int \chi_q^*(\underline{r})\ k^2\ \chi_s(\underline{r})\ d\tau = \langle q|k^2|s\rangle \tag{13}$$

$$\int \chi_q^*(\underline{r}_1)\ \chi_r^*(\underline{r}_2)\ \underline{r}_1\cdot\underline{r}_2\ \chi_s(\underline{r}_1)\ \chi_t(\underline{r}_2)\ d\tau_1\ d\tau_2 = \langle qr|\underline{r}_1\cdot\underline{r}_2|st\rangle$$

$$\int \chi_q^*(\underline{r}_1)\ \chi_r^*(\underline{r}_2)\ \underline{k}_1\cdot\underline{k}_2\ \chi_s(\underline{r}_1)\ \chi_t(\underline{r}_2)\ d\tau_1\ d\tau_2 = \langle qr|\underline{k}_1\cdot\underline{k}_2|st\rangle$$

$$\int \chi_q^*(\underline{r}_1)\ \chi_r^*(\underline{r}_2)\ V_{12}'\ \chi_s(\underline{r}_1)\ \chi_t(\underline{r}_2)\ d\tau_1\ d\tau_2 = \langle qr|V_{12}'|st\rangle \quad .(14)$$

In order to evaluate the matrix elements of k^2 and $\underline{k}_1\cdot\underline{k}_2$, it is convenient to write the wavefunctions χ in k-space. Denoting the general point in k-space as $(k_\rho,\ \phi_k,\ k_z)$, the harmonic oscillator function χ_{n,m,n_z} (3) transforms into:

$$\Omega_{n,m,n_z}(k_\rho,\phi_k,k_z) = (2\pi)^{-\frac{3}{2}} \int e^{ik.\underline{r}}\ \chi_{n,m,n_z}(\sqrt{\alpha}\rho,\phi,\sqrt{a}z)\,\rho d\rho d\phi dz.$$

This integral can be evaluated$^{(9)}$ to give:

$$\Omega_{n,m,n_z} = i^{2n+|m|+n_z}\ P_{n,m}(\sqrt{\alpha^{-1}}\ k_\rho)\ \Phi_m(\phi_k)\ Z_{n_z}(\sqrt{a^{-1}}\ k_z).(15)$$

Thus, apart from the phase factor, $i^{2n+|m|+n_z}$, Ω is obtained by replacing α and a everywhere by their inverses, and substituting k_ρ for ρ, etc. This will prove to be very useful in the evaluation of matrix elements.

Following Manning$^{(10)}$, we now define the following integrals:

$$R_{qs}^{(n)} = \int_0^\infty P_{n_q,m_q}(\sqrt{\alpha}\ \rho)\ \rho^n\ P_{n_s,m_s}(\sqrt{\alpha}\ \rho)\ \rho d\rho \qquad n=0,1,2,\ldots$$

$$R_{qs}^{(-n)} = \int_0^\infty P_{n_q m_q}(\sqrt{\alpha^{-1}}\ k_\rho)\ k_\rho^n\ P_{n_s m_s}(\sqrt{\alpha^{-1}}\ k_\rho)\ k_\rho\ dk_\rho \quad n=1,2,\ldots$$

$$Z_{qs}^{(n)} = \int_{-\infty}^\infty Z_{n_{z_q}}(\sqrt{a}\ z)\ z^n\ Z_{n_{z_s}}(\sqrt{a}\ z)\ dz \qquad n=0,1,2,\ldots$$

$$Z_{qs}^{(-n)} = \int_{-\infty}^\infty Z_{n_{z_q}}(\sqrt{a^{-1}}\ k_z)\ k_z^n\ Z_{n_{z_s}}(\sqrt{a^{-1}}\ k_z)\ dk_z \qquad n=1,2,\ldots \tag{16}$$

Matrix elements for all operators (except the two-body potential energy) in the Hamiltonian (9) can be expressed in terms of the above integrals. (The explicit forms for these integrals are developed in Appendix A.) It is clear that

$$\langle q|\rho^2|s\rangle = \delta_{m_q,m_s}\ R_{qs}^{(2)}\ Z_{qs}^{(0)} \qquad ,$$

and

$$\langle q|z^2|s\rangle = \delta_{m_q,m_s}\ R_{qs}^{(0)}\ Z_{qs}^{(2)} \qquad ,$$

whence

$$\langle q|r^2|s\rangle = \delta_{m_q,m_s}\{R_{qs}^{(2)}\ Z_{qs}^{(0)} + R_{qs}^{(0)}\ Z_{qs}^{(2)}\} \tag{17}$$

In order that this matrix element be non-zero, it is also necessary that the parities of states q and s be the same. In k-space:

$$<q|k^2|s> = \delta_{m_q,m_s}\{i^{2n_s-2n_q+|m_s|-|m_q|} R_{qs}^{(-2)} Z_{qs}^{(0)} + i^{n_{z_s}-n_{z_q}}$$

$$\times R_{qs}^{(0)} Z_{qs}^{(-2)}\} \qquad .(18)$$

Again, the parities of states q and s must be the same, and when both the parity and m selection rules are satisfied, the complex factors reduce to ±1.

The evaluation of the two-body matrix elements is more difficult

$$<qr|\underline{r}_1\cdot\underline{r}_2|st> = <qr|\rho_1\rho_2 \cos(\phi_1-\phi_2)|st> + <qr|z_1z_2|st>.$$

The integrations over the ϕ's in each term are easy, and give factors of $\frac{1}{2}\,\delta_{m_q-m_s,\pm1}\,\delta_{m_r-m_t,\mp1}$ and $\delta_{m_q,m_s}\,\delta_{m_r,m_t}$ respectively. As well, in order for the matrix elements to be non-zero, the parities of q and s must be opposite (similarly for r and t). The remaining integrals over the ρ's and z's separate into integrals of the form (16). The result is:

$$<qr|\underline{r}_1\cdot\underline{r}_2|st> = \tfrac{1}{2}\,\delta_{m_q-m_s,\pm1}\,\delta_{m_r-m_t,\mp1}\,R_{qs}^{(1)}\,R_{rt}^{(1)}\,Z_{qs}^{(0)}\,Z_{rt}^{(0)}$$

$$+ \delta_{m_q,m_s}\,\delta_{m_r,m_t}\,R_{qs}^{(0)}\,R_{rt}^{(0)}\,Z_{qs}^{(1)}\,Z_{rt}^{(1)} \qquad .(19)$$

Similarly, in k-space:

$$\langle qr|\underline{k}_1 \cdot \underline{k}_2|st\rangle = \tfrac{1}{2}\, \delta_{m_q-m_s,\pm 1}\, \delta_{m_r-m_t,\mp 1}$$
$$\times\ i^{(2n_s+2n_t-2n_q-2n_r+|m_s|+|m_t|-|m_q|-|m_r|)}$$
$$\times\ R^{(-1)}_{qs}\ R^{(-1)}_{rt}\ Z^{(0)}_{qs}\ Z^{(0)}_{rt} + \delta_{m_q,m_s}\, \delta_{m_r,m_t}$$
$$\times\ i^{(n_{z_s}+n_{z_t}-n_{z_q}-n_{z_r})}\ R^{(0)}_{qs}\ R^{(0)}_{rt}\ Z^{(-1)}_{qs}\ Z^{(-1)}_{rt} \qquad .(20)$$

When the parity and m conditions are met, the phase factors are ±1.

Thus, by using expressions (17) through (20), all matrix elements may be evaluated, with the exception of those involving the two-body potential operator. These matrix elements may be determined by using formulae developed by Copley and Volkov(11). Since these formulae are rather lengthy, they are written in Appendix B. Thus, we now have expressions for all desired matrix elements and the Hamiltonian matrix may easily be constructed and diagonalized.

Electric Quadrupole Transitions

As in the two-particle problem, we want to determine the B(E2)'s and T(E2)'s (defined by (I-22) and (I-21)) for transitions between eigenstates. Following the procedure adopted in Chapter I, we calculate one matrix element of the form $<f|Q_{20}|i>$, where $M_f = M_i$, from which we can determine the RME, and hence all other matrix elements of the form $<f|Q_{2u}|i>$. Now the problem is to determine

$$<\psi^f|Q_{20}|\psi^i> = \sum_k \sum_\ell c_k^f \, c_\ell^i \, <\psi_k|Q_{20}|\psi_\ell> \quad .$$

Q_{20} is a one-body operator:

$$Q_{20} = \sum_{i=1}^{3} e_i \, (3z_i^2 - r_i^2)$$

$$= e \sum_{i=1}^{3} (2z_i^2 - \rho_i^2) \quad .$$

Therefore in order for $<\psi_k|Q_{20}|\psi_\ell>$ to be non-zero, we must have two of the single-particle states in ψ_k the same as two of the single-particle states in ψ_ℓ. If this is satisfied, the matrix element reduces to a sum of matrix elements of the form:

$$<q|2z^2-\rho^2|s> = \delta_{m_q,m_s} [2 \, R_{qs}^{(0)} \, Z_{qs}^{(2)} - R_{qs}^{(2)} \, Z_{qs}^{(0)}] \quad .$$

Thus, it is quite easy to determine $<\psi^f|Q_{20}|\psi^i>$, and then the B(E2) and T(E2).

CHAPTER III

COMPUTATION

Computation was performed on a CDC 6400 computer. For the most part, the programmes were developed straightforwardly from expressions in Chapters I and II. For matrix diagonalization, the library subroutine HOUSE 4 was used; this uses Householder's method to tridiagonalize the matrix and then the Ortega method to find the eigenvalues and eigenvectors. For the two-particle problem, a basis of 80 states was used, and hence the matrix which was required to be diagonalized was 80 x 80. This size of basis was deemed to be large enough for several reasons:

(a) The eigenvectors and eigenvalues for the lowest eigenstates (ie. the bound ones) remained unchanged to 6 significant figures if a larger basis was used.

(b) Our results were compared with results from an accurate numerical solution of the Schrodinger equation and found to agree to 6 significant figures.

(c) The eigenvalues and eigenvectors of the bound states were unchanged (6 figures) with a change of oscillator constant of 15%.

Using an 80-state basis, the time taken to generate the matrix elements for a given J and diagonalize the matrix was typically of the order of 1 min. (which is quite fast). This includes also the calculation of $<r^2>$ (an expression for which is obtained trivially by using Eq. (I-17)) for each of the bound eigenstates.

In the case of three particles, the matrices involved can become very large. Table 1 shows the sizes of the matrices for the possible excitations ($2\hbar\omega$, $4\hbar\omega$, ...etc.) out of the basis ground state, for the various M-values. Also tabulated are the matrix sizes (ie. basis sizes) that would exist if the particles were coupled to a definite J. (The matrix size for a given J is of course simply equal to the matrix for M = J-1 minus the matrix size for M=J.)

From Table 1, it is clear that even for excitations as low as $8\hbar\omega$, the matrices are getting extremely large for the lower M-values. The largest matrix which was feasible for calculation purposes was 231 x 231 ($8\hbar\omega$, M=3). For this matrix, it was necessary to employ overlays in the computer programme, since it was impossible to store the matrix and at the same time retain in core all the subroutines necessary to generate the matrix. Even with overlays, the programme required all of the machine's core (124000_8). The time necessary to generate and diagonalize the matrix was 33 min. For matrices of sides 117 ($6\hbar\omega$, M=0) and 49 ($6\hbar\omega$, M=3), the corresponding times were 6 and 1 min., respectively. Thus, it is seen that as the size of the

TABLE 1

DIMENSIONALITIES OF MATRICES IN THREE-PARTICLE PROBLEM

EXCITATION ABOVE BASIS GROUND STATE:

	$2\hbar\omega$		$4\hbar\omega$		$6\hbar\omega$		$8\hbar\omega$		$10\hbar\omega$		$12\hbar\omega$	
M or J	S_M	S_J	S_M	S_J	S_M	S_J	S_M	S_J	S_M	S_J	S_M	S_J
0	5	3	27	9	117	23	413	51	1241	103	3282	196
1	2	0	18	2	94	10	362	34	1138	90	3086	206
2	2	2	16	10	84	35	328	97	1048	231	2880	489
3			6	2	49	15	231	57	817	165	2391	399
4			4	4	34	22	174	80	652	224	1992	534
5					12	5	94	35	428	131	1458	369
6					7	7	59	39	297	143	1089	403
7							20	10	154	64	686	234
8							10	10	90	60	452	223
9									30	16	229	101
10									14	14	128	86
11											42	23
12											19	19

S_M: Matrix size for particles coupled to definite M.

S_J: Matrix size for particles coupled to definite J.

(matrix size = number of 3-particle basis states) matrix increases, the time required increases greatly; the matrix storage space required in the machine also increases tremendously, varying as the square of the matrix size.

One of the most time-consuming parts of the three-particle programme was the calculation of the two-body potential matrix elements. It was decided that since many matrix elements $\langle qr|V'|st\rangle$ are required several times, the matrix elements should be stored when calculated, so that the next time this particular matrix element is required, it can be quickly picked out of the stored array rather than being recalculated. In fact, to further save time, the radial and angular part, and the z-part of the matrix element were stored separately, since a particular radial and angular part, for example, can be common to several total matrix elements which have different z-parts. As well, many matrix elements are equivalent, eg. $M_{qrst} = M_{rqts} = M_{stqr} = M_{tsrq}$, where M_{qrst} is the radial and angular part of the matrix element between states q and r, and s and t. This feature was taken into account in the calculation and storage of the matrix elements. Time reversal symmetry was also employed, ie. the fact that

$$M_{q_{m_q} s_{m_s} r_{m_r} t_{m_t}} = M_{q_{-m_q} s_{-m_s} r_{-m_r} t_{-m_t}}$$

was taken into account.

Thus, whenever a potential matrix element is to be calculated, a search is made to determine whether the radial and angular, and/or z-parts have already been calculated and stored. If so, the matrix element can be quickly determined; if not, it must be calculated and stored. This saves considerable time, but of course requires one-dimensional arrays in which to store previously calculated matrix elements. The arrays for the z-parts are small (the largest used had a size of 150), but for the radial and angular parts, the arrays were as large as 1175. Two arrays (for the attractive and repulsive part of the potential) were required for each of the radial and angular, and z-parts.

CHAPTER IV

RESULTS, DISCUSSION AND CONCLUSIONS

Two Particle Results

Four different two-body potentials (Table II and Fig. 2) were used, ranging from that of a soft rotor (potential I) to that of a hard one (potential IV).

TABLE II

POTENTIAL PARAMETERS

Potential	V'_a	V'_r	K_a	K_r
	units of μc^2		units of $(\frac{\mu c}{\hbar})^2$	
I	-15.00	11.25	.0165	.0330
II	-17.00	15.50	.0165	.0330
III	-25.00	38.30	.0204	.0408
IV	-50.00	76.60	.0204	.0408

Energy levels for the lowest states for each potential are shown in Figs. 3-6. The levels have been divided into rotational-vibrational bands, as might be observed experimentally. Clearly, as the potential becomes harder, the

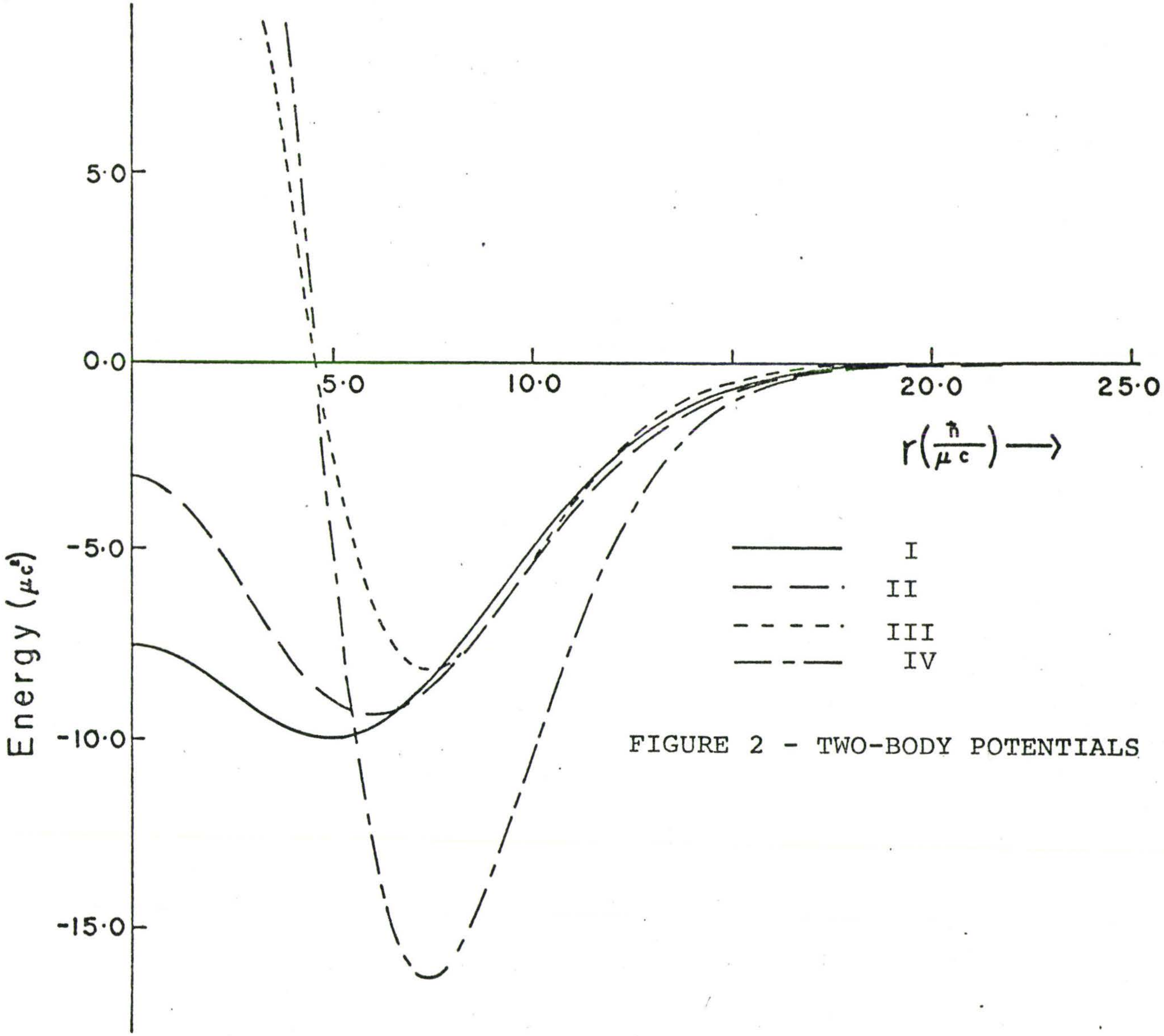


FIGURE 2 - TWO-BODY POTENTIALS

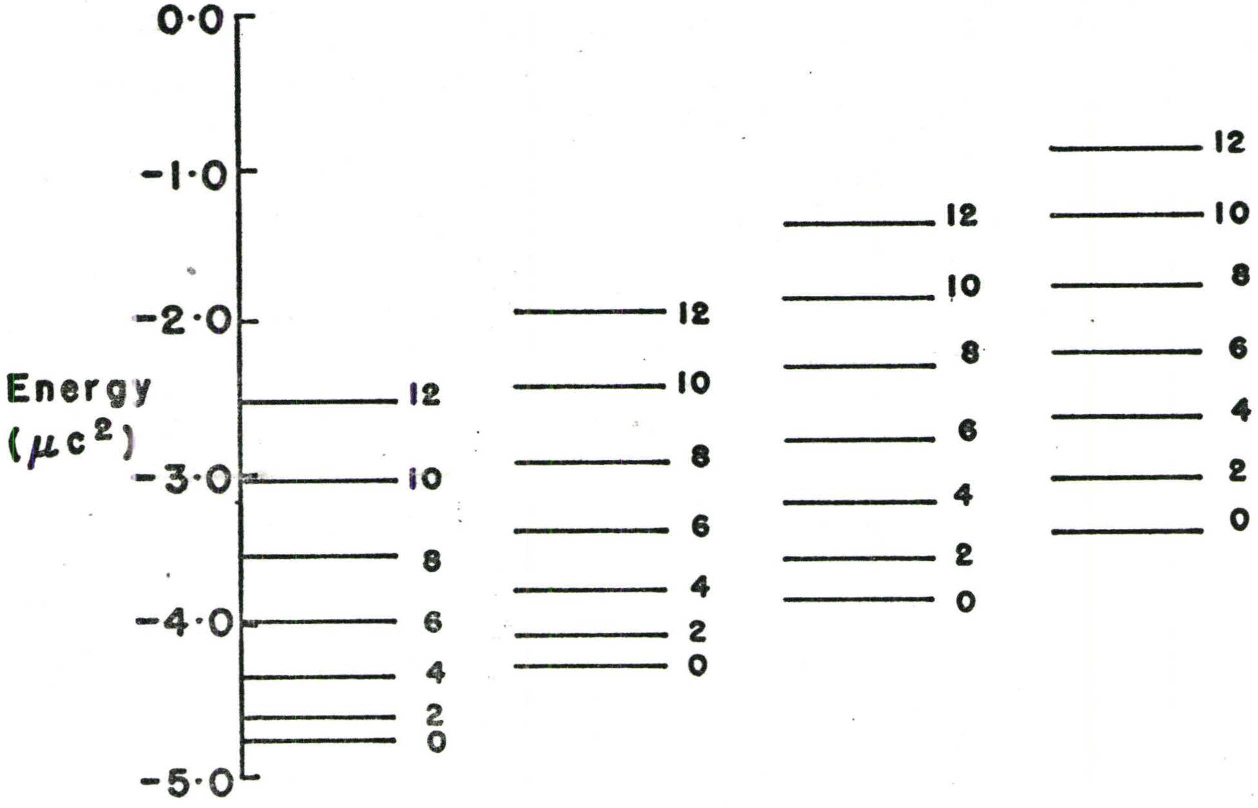


FIGURE 3 - ENERGY LEVELS FOR POTENTIAL I

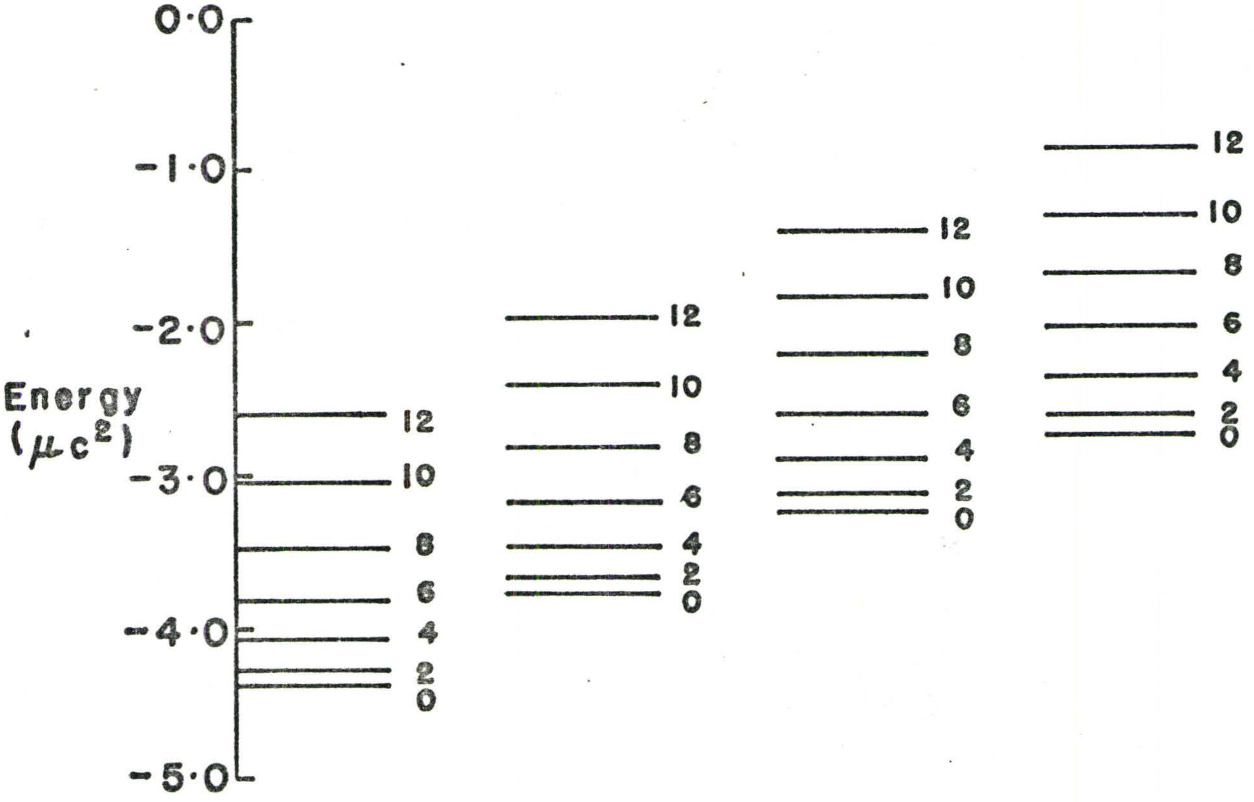


FIGURE 4 - ENERGY LEVELS FOR POTENTIAL II

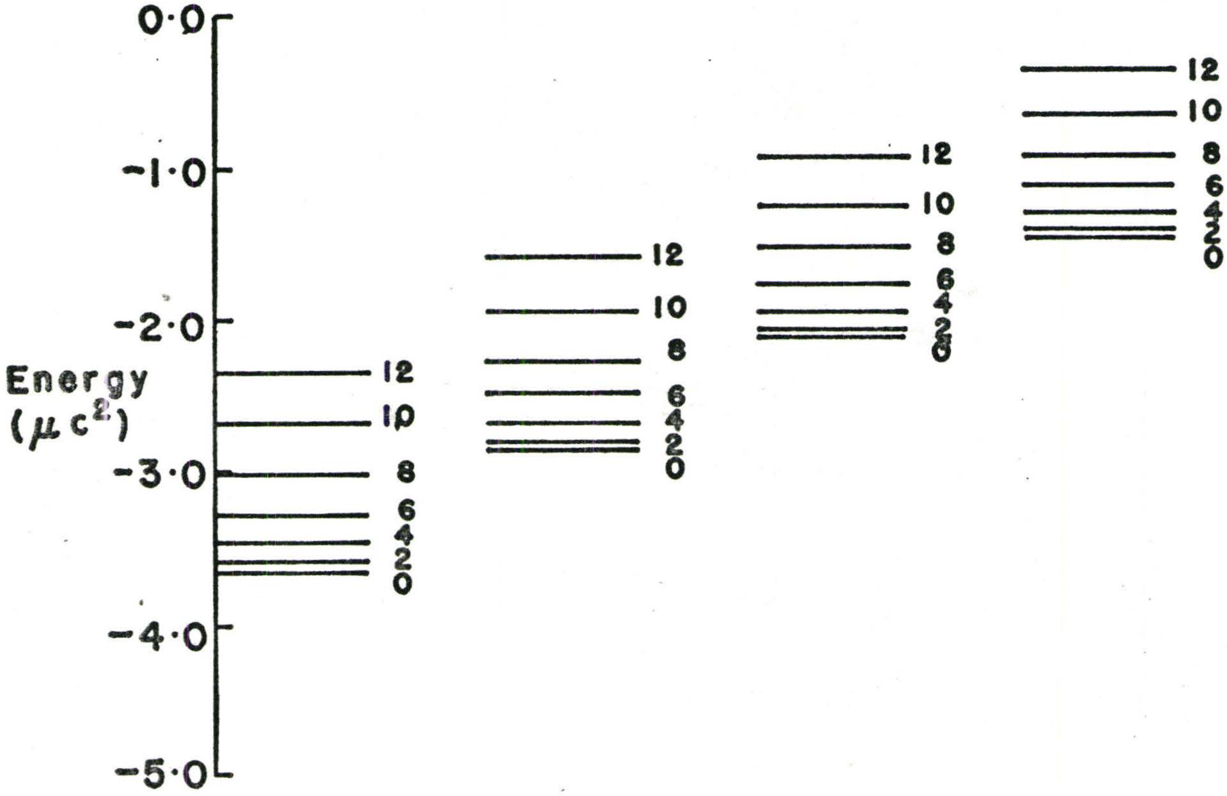


FIGURE 5 - ENERGY LEVELS FOR POTENTIAL III

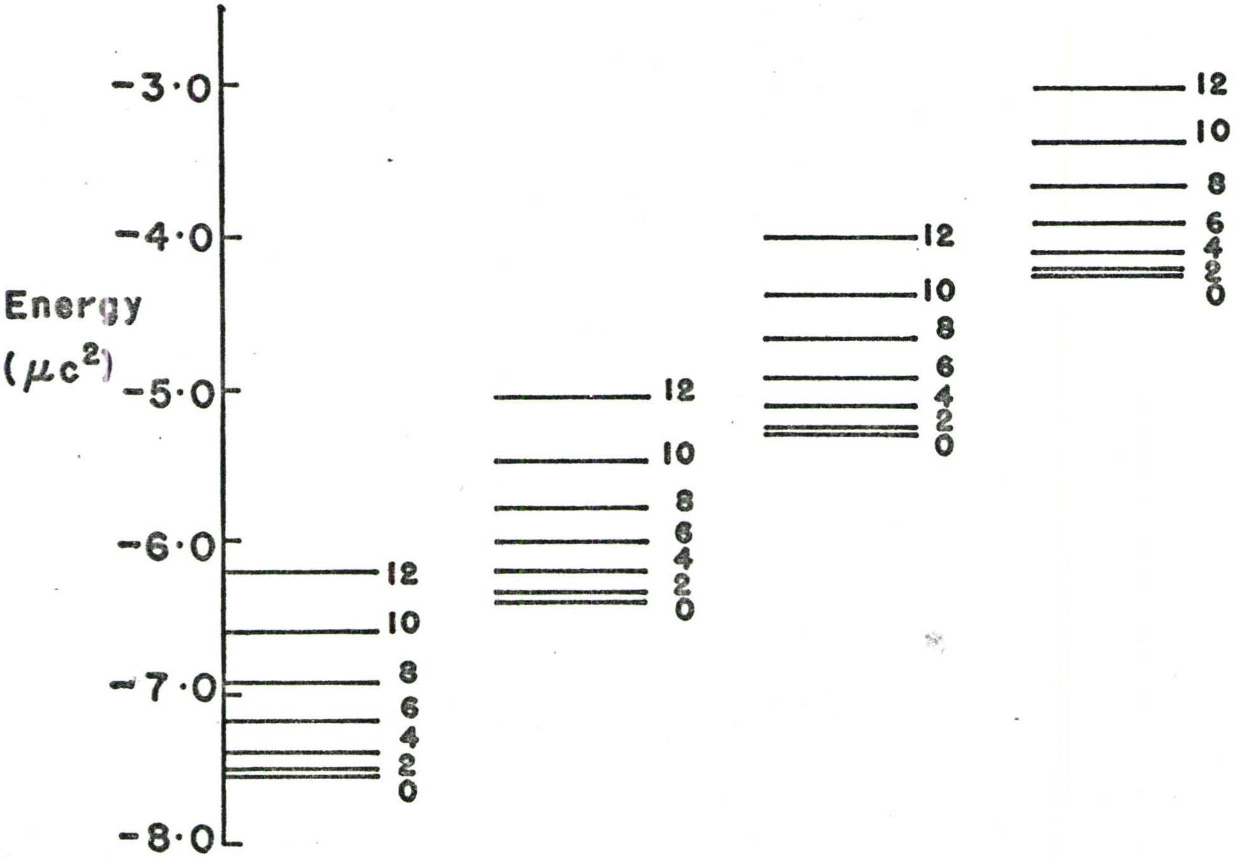


FIGURE 6 - ENERGY LEVELS FOR POTENTIAL IV

energies associated with the rotational and vibrational motions differ more and more. In the case of a very hard potential (ie. much harder than potential IV) such as in a molecule, the various bands are well separated in energy.

There are several justifications for separating the resulting eigenstates into bands. First is the form of the radial wavefunctions in the various bands. In the lowest band (for any potential), the radial wavefunctions have no nodes; in the second band, the radial wavefunctions have one node, and so on. Thus, the radial form of the wavefunction clearly distinguishes various bands. In Figs. 7 and 8, this is shown quite explicitly: $|\psi_r|^2 r^2$ is plotted against r for potentials I and III for the J=0 states in the three lowest bands, where ψ_r is the radial wavefunction. As well, the values of $\langle r^2 \rangle$ are shown for each of these wavefunctions. Clearly as one goes from band to band, the value of $\langle r^2 \rangle$ changes; this indicates stretching of the two-particle system as it goes from a lower vibrational mode to a higher one. We might also expect stretching to occur within a band, as the rotational energy increases. In fact, we find this, as is shown in Figs. 9 and 10, where $|\psi_r|^2 r^2$ is shown for the J=0, 6, and 12 states of the lowest band in potentials I and III. Note that the stretching is much less for the harder potential (III), which is to be expected. For a rigid rotor, one expects a strict J(J+1) dependence in the energy levels. However, the stretching

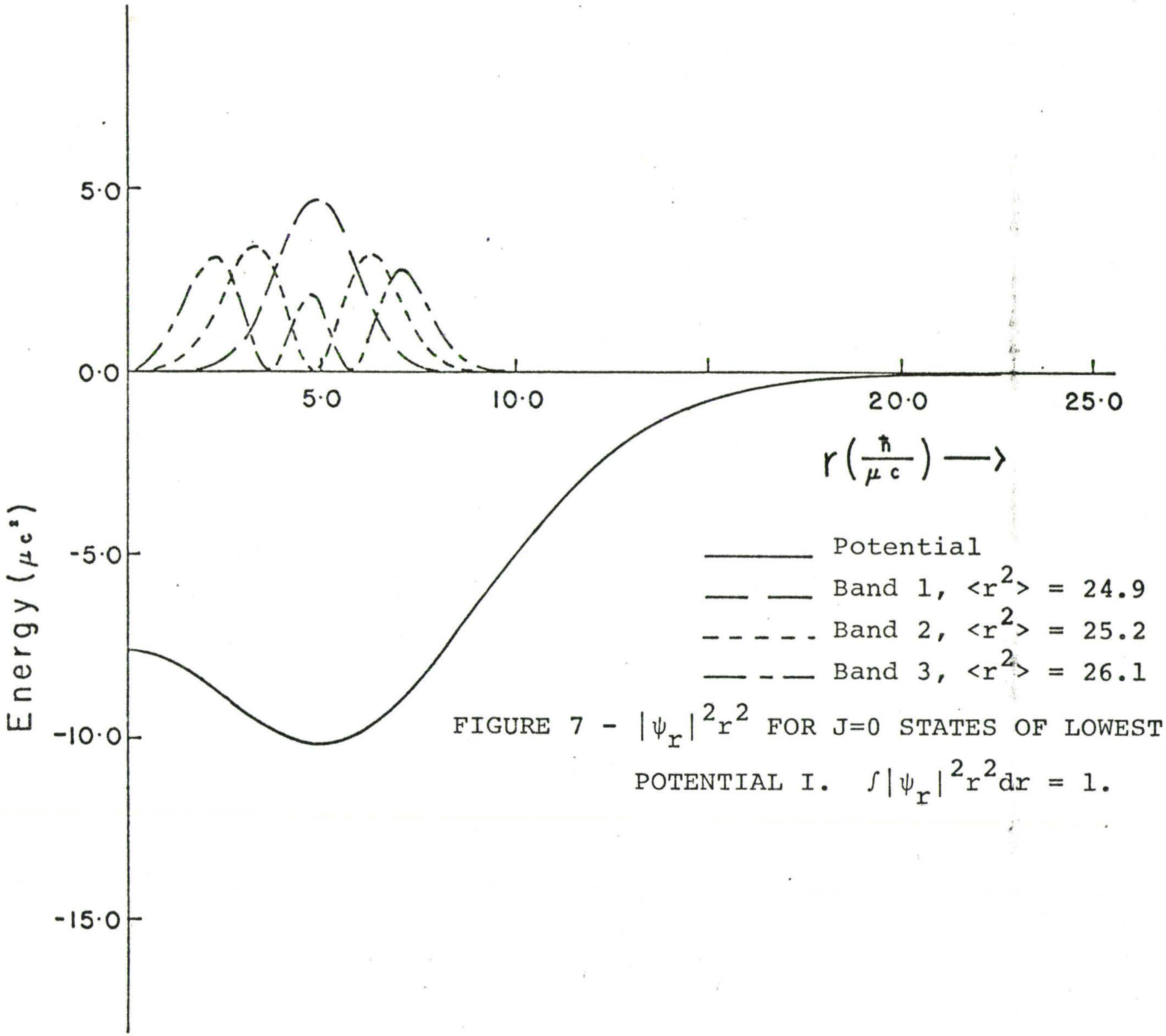


FIGURE 7 - $|\psi_r|^2r^2$ FOR J=0 STATES OF LOWEST 3 BANDS IN POTENTIAL I. $\int|\psi_r|^2r^2dr = 1$.

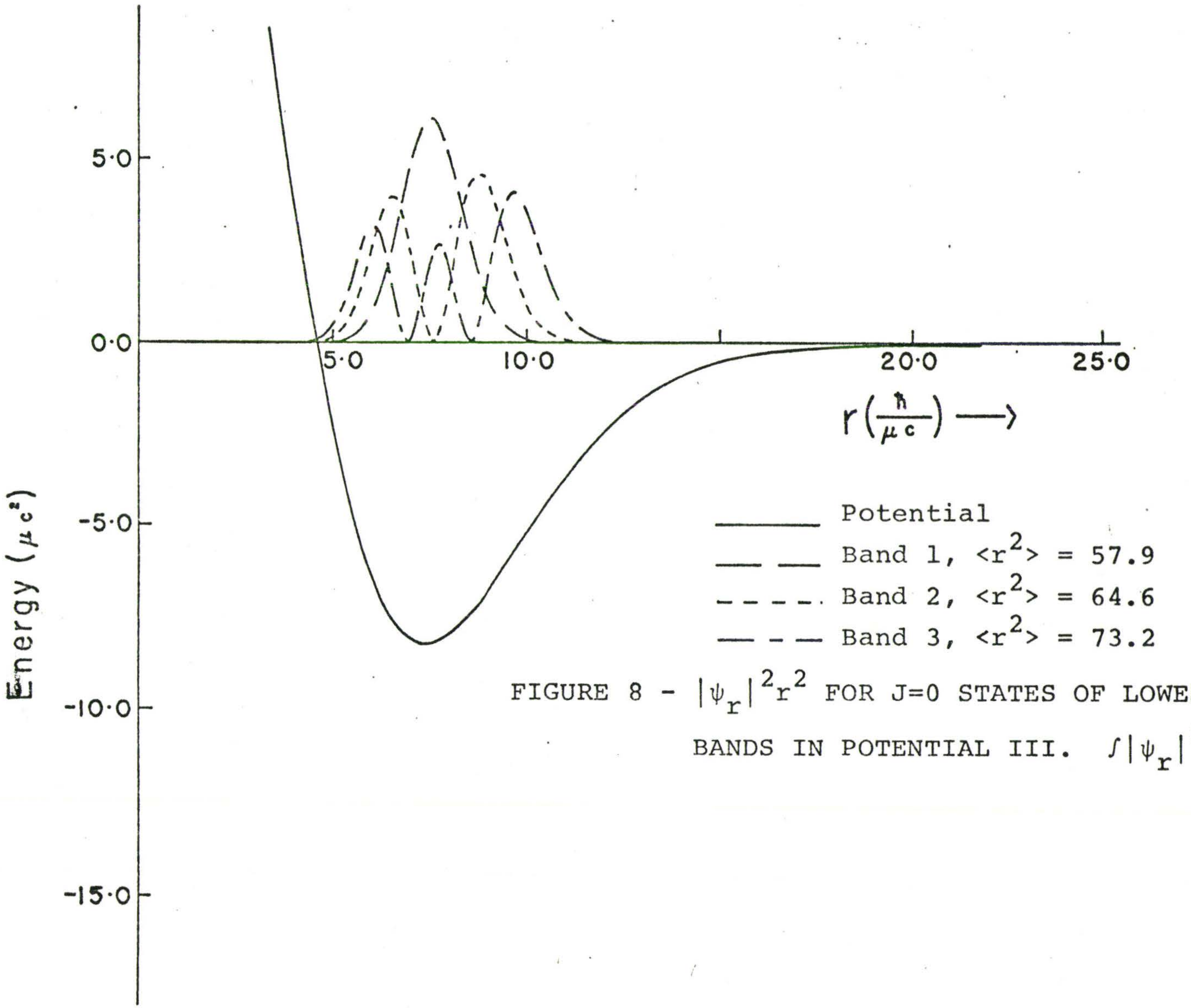


FIGURE 8 - $|\psi_r|^2 r^2$ FOR J=0 STATES OF LOWEST 3 BANDS IN POTENTIAL III. $\int |\psi_r|^2 r^2 dr = 1$.

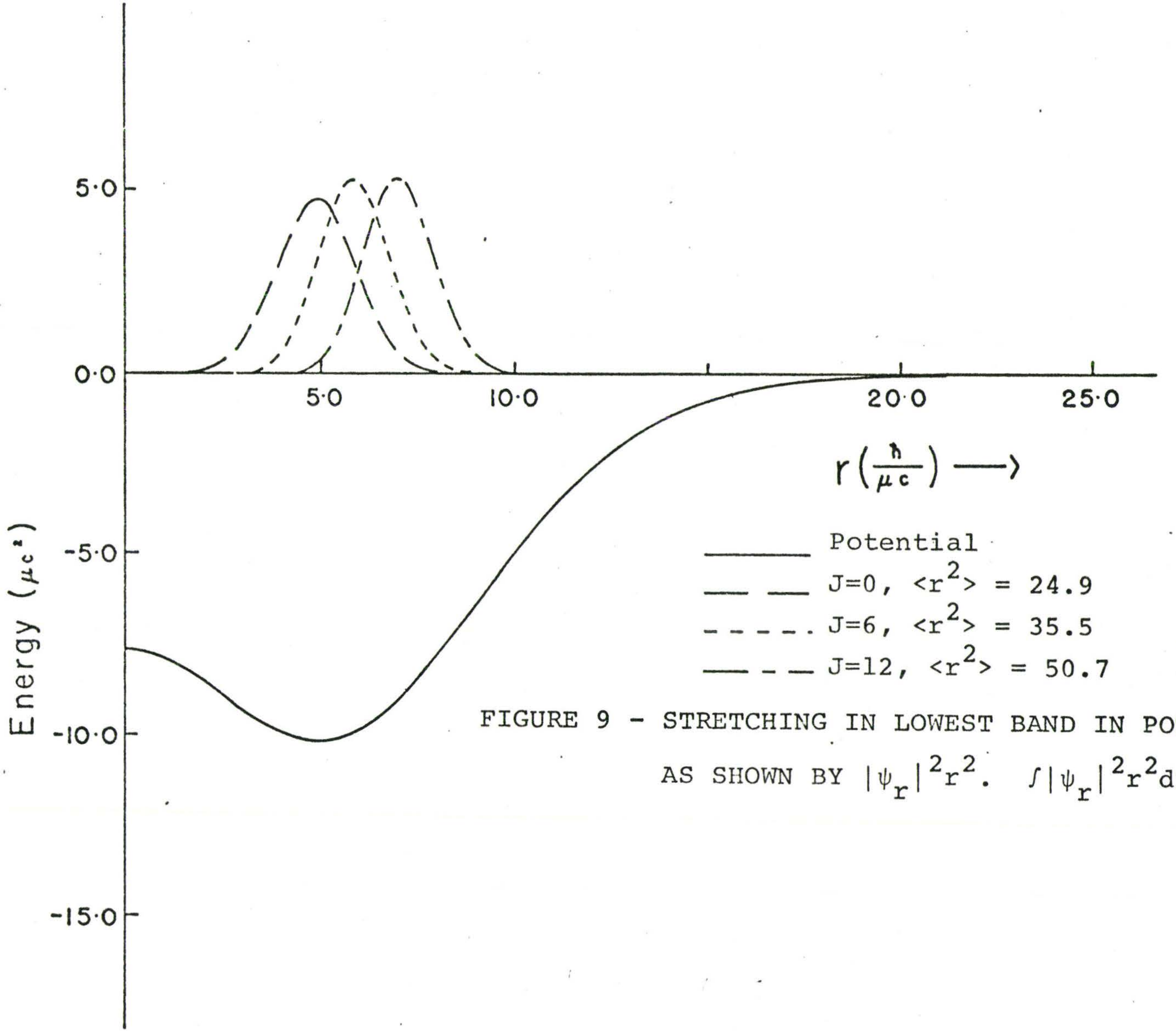


FIGURE 9 - STRETCHING IN LOWEST BAND IN POTENTIAL I, AS SHOWN BY $|\psi_r|^2 r^2$. $\int |\psi_r|^2 r^2 dr = 1$.

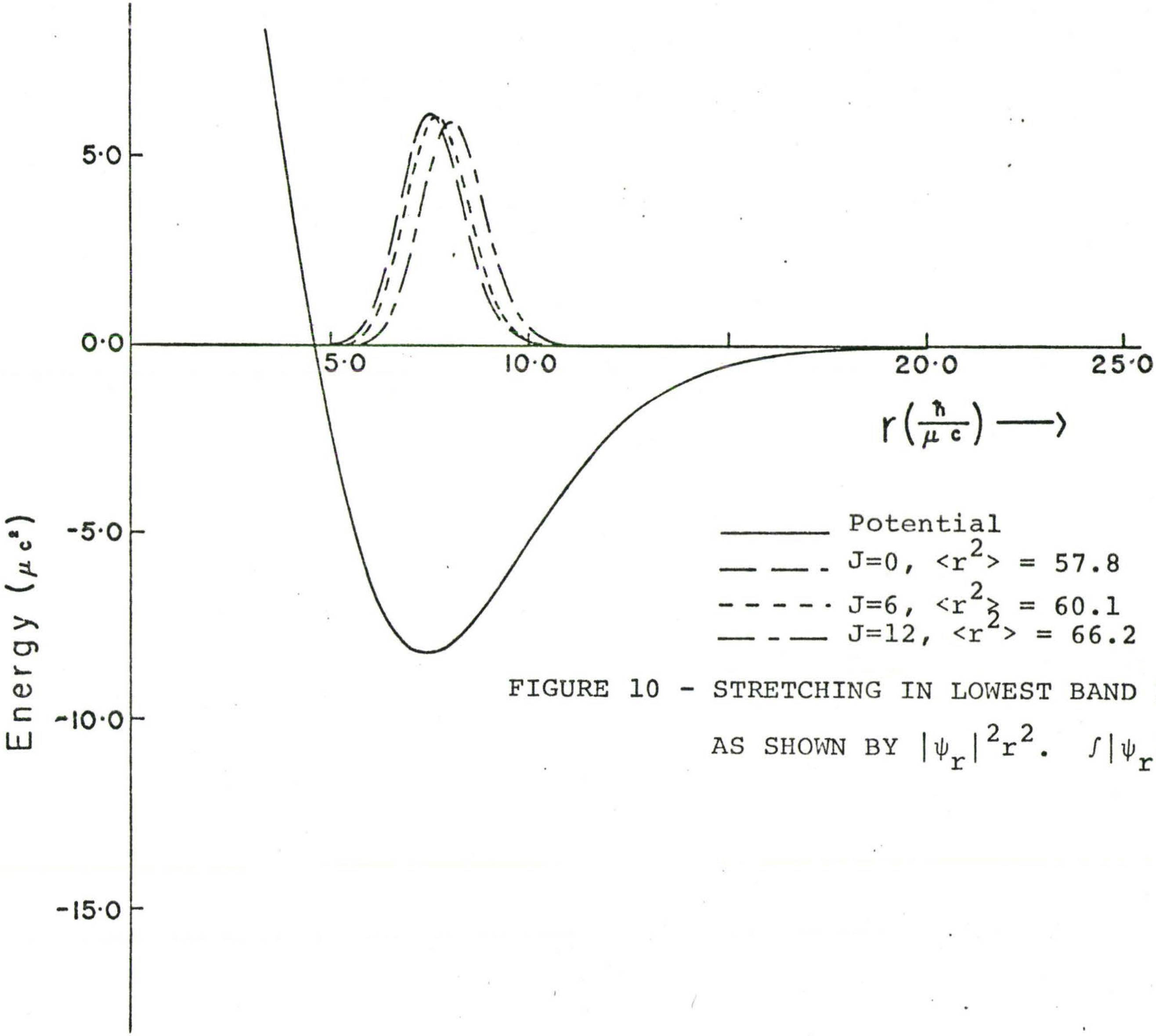
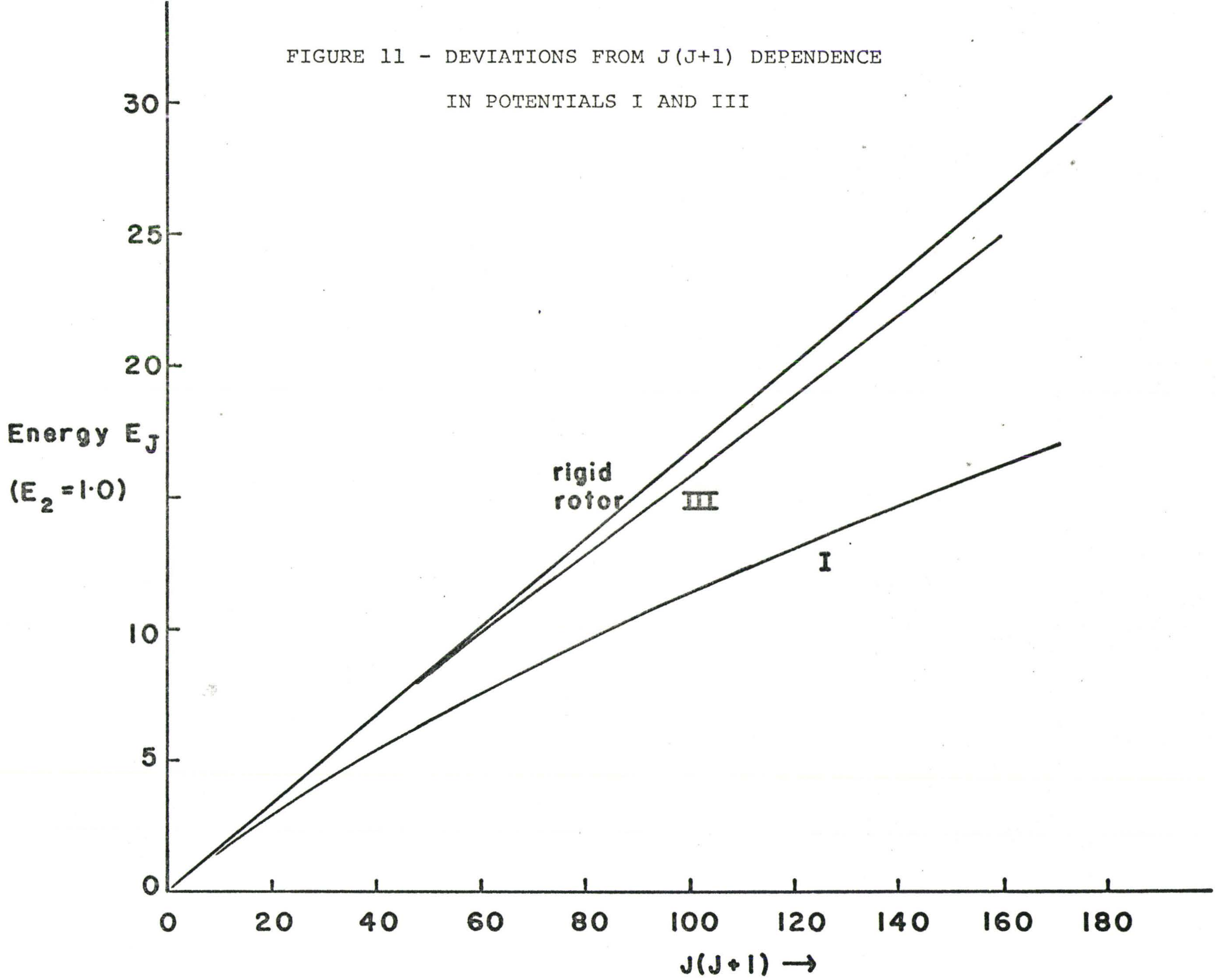


FIGURE 10 - STRETCHING IN LOWEST BAND IN POTENTIAL III, AS SHOWN BY $|\psi_r|^2 r^2$. $\int |\psi_r|^2 r^2 dr = 1$.

FIGURE 11 - DEVIATIONS FROM J(J+1) DEPENDENCE IN POTENTIALS I AND III



just noted will destroy this dependence to some extent, and it would be expected that the greater the stretching, the greater the deviations from the J(J+1) dependence. This is shown in Fig. 11, where the deviations from J(J+1) dependence for the lowest band of potential I (large stretching) are seen to be much greater than those for the lowest band of potential III (small stretching). Note in Fig. 11 that the energy of the J=2 state has been set equal to 1.0 for each of the three cases (rigid rotor, potentials I and III). The energy levels for a rigid rotor are $\frac{A}{I}$ J(J+1), where I is the moment of inertia of the object. In the case of a non-rigid rotor, we would expect the moment of inertia to increase as the object stretches with increasing angular momentum, and thus the energies of states of higher J are less than what would be expected for a rigid rotor. This is indeed what is shown in Fig. 11.

Another justification for separating the eigenstates into bands is the fact that the B(E2)'s for transitions within a band are greater than those for transitions between bands (as is observed experimentally in axially symmetric even-even nuclei with rotational spectra). This is seen in Figs. 12 and 13, where a few representative B(E2)'s have been indicated for transitions between states in potentials I and III. These B(E2)'s are not in fact exactly those B(E2)'s defined by Eq. (I-22); since the relative magnitudes only are of importance, we have set the charge e on each

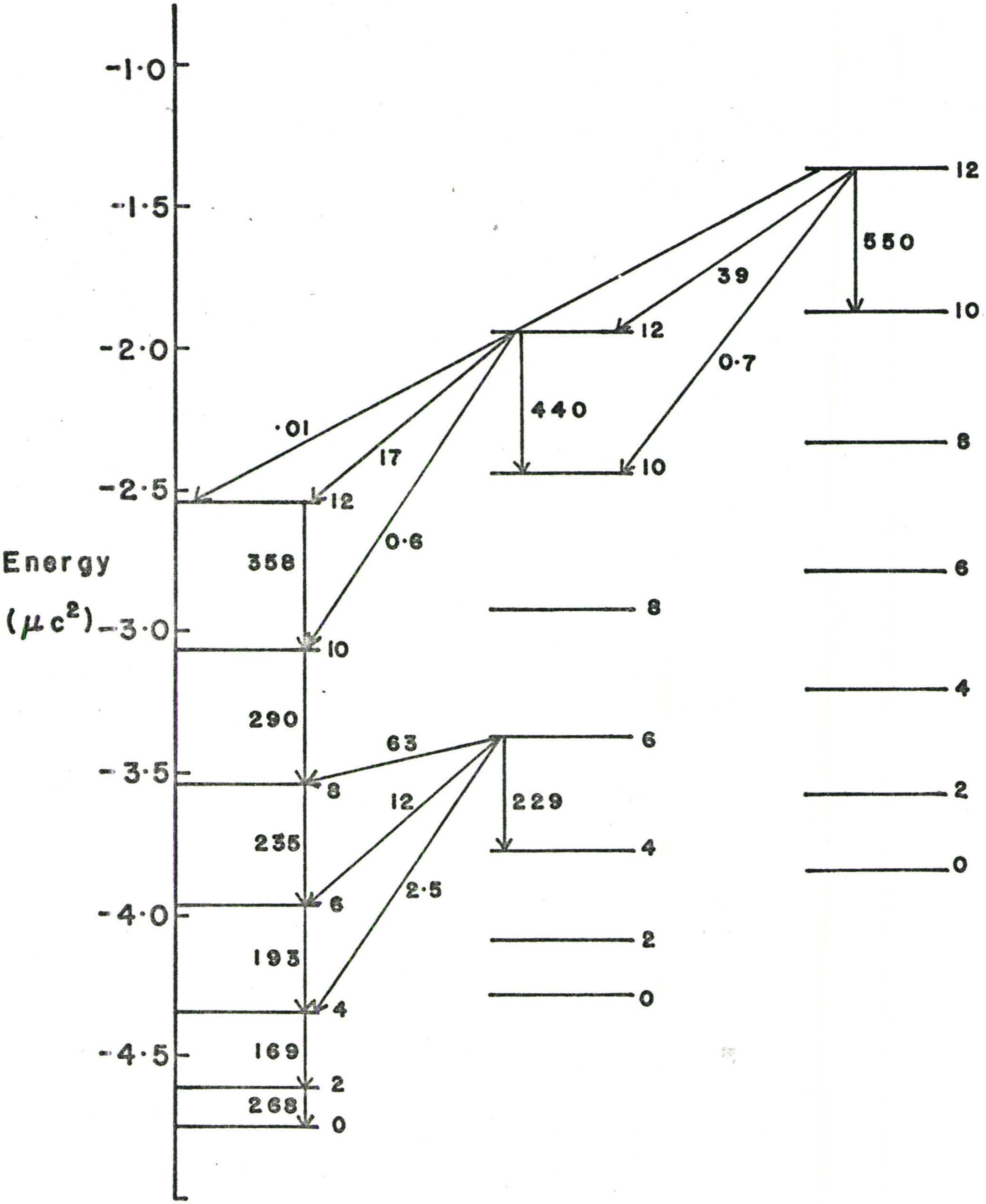


FIGURE 12 - B(E2)'s FOR TRANSITIONS BETWEEN STATES IN POTENTIAL I

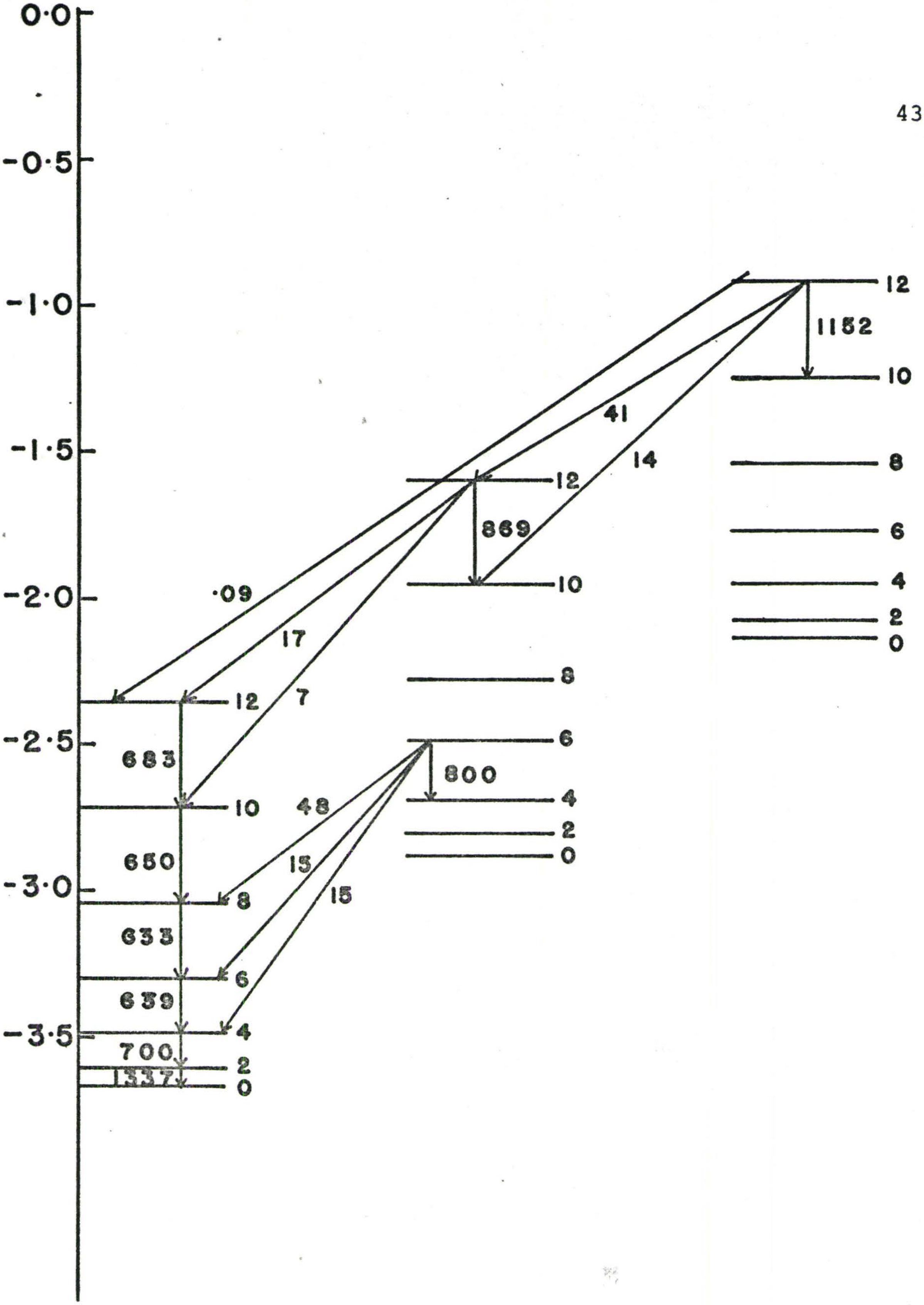


FIGURE 13 - B(E2)'s FOR TRANSITIONS BETWEEN STATES IN POTENTIAL III

particle equal to 1. Note in Figs. 12 and 13 that the B(E2)'s for in-band transitions are at least a factor of 10 larger than those for cross-band transitions.

It is also interesting to investigate whether we get the so-called "Yrast" levels. To do this, we assume that we have populated the J=10 state in the third band (for potentials I and III), and calculate the probabilities of populating the lower states as the system decays. The results are shown in Table III. We clearly have the occurrence of Yrast levels, which are much more prominent in the case of the harder potential (III). In this case, they are the J=8 level in the second band and all the levels for J<6 in the first band.

Three-Particle Results

Unfortunately, the results for the three-particle problem are not as satisfactory as those for the two-particle case. The general procedure followed was to construct all basis states representing an excitation of no more than $2\hbar\omega$ above the basis ground state, and then to perform the calculation using this basis; then a basis of states representing no more than a $4\hbar\omega$ excitation was used, and so on, until the eigenvalues and eigenvectors did not change when the basis was increased -- unhappily, this point was never reached. Figs. 14 and 15 show the energy levels for states (with no centre-of-mass excitation)

TABLE III

POPULATION PROBABILITIES

(a) Potential 1

		band		
		1	2	3
J	12	.03	<.01	0.00
	10	.02	.15	1.00
	8	.09	.37	.72
	6	.28	.49	.42
	4	.56	.40	.17
	2	.86	.18	.04
	0	1.00	.03	< .01

(b) Potential III

		band		
		1	2	3
J	12	.01	.02	0.00
	10	.11	.21	1.00
	8	.50	.63	.07
	6	.95	.06	< .01
	4	1.00	<.01	< .01
	2	1.00	<.01	< .01
	0	1.00	<.01	< .01

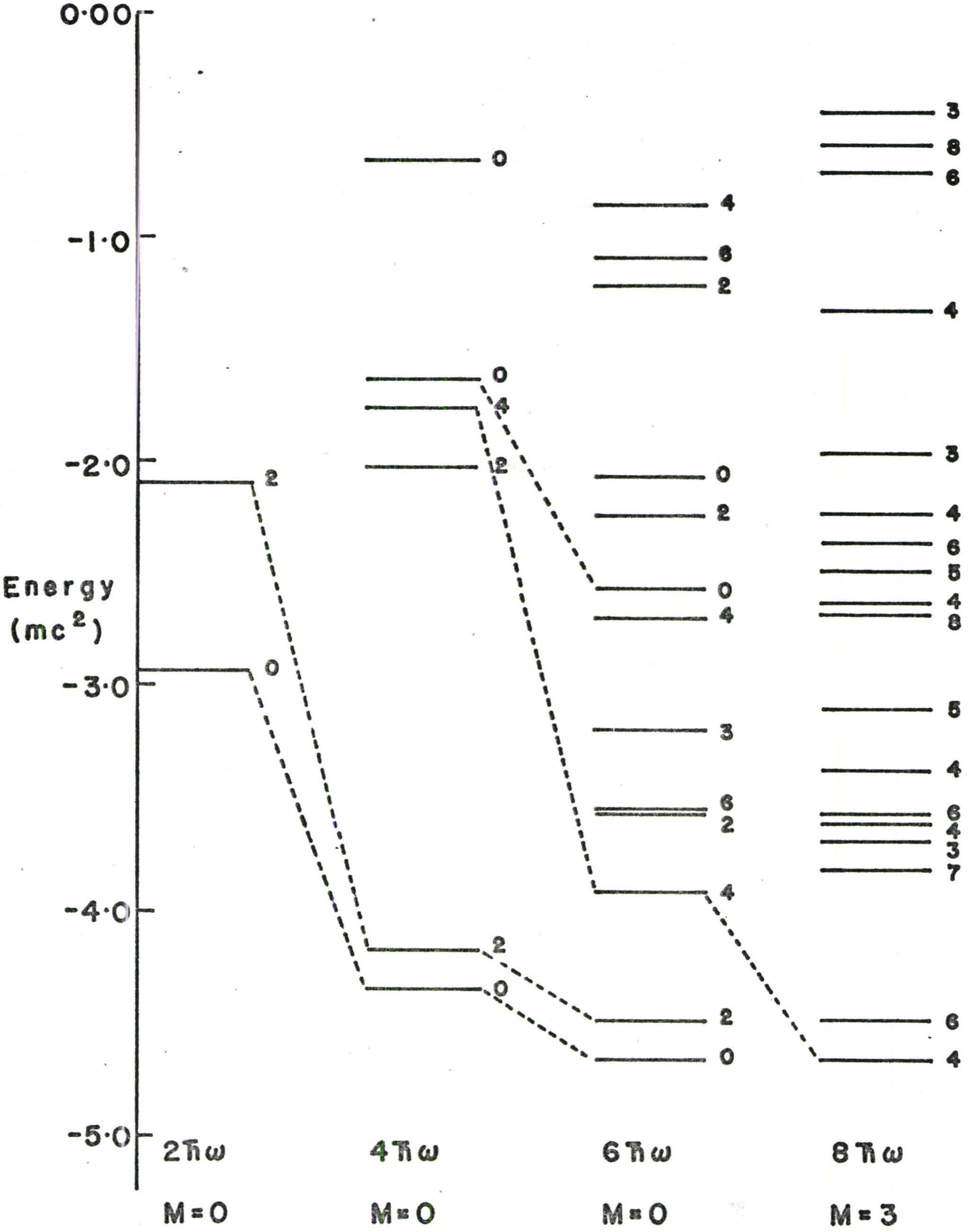


FIGURE 14 - ENERGY LEVELS FOR POTENTIAL III

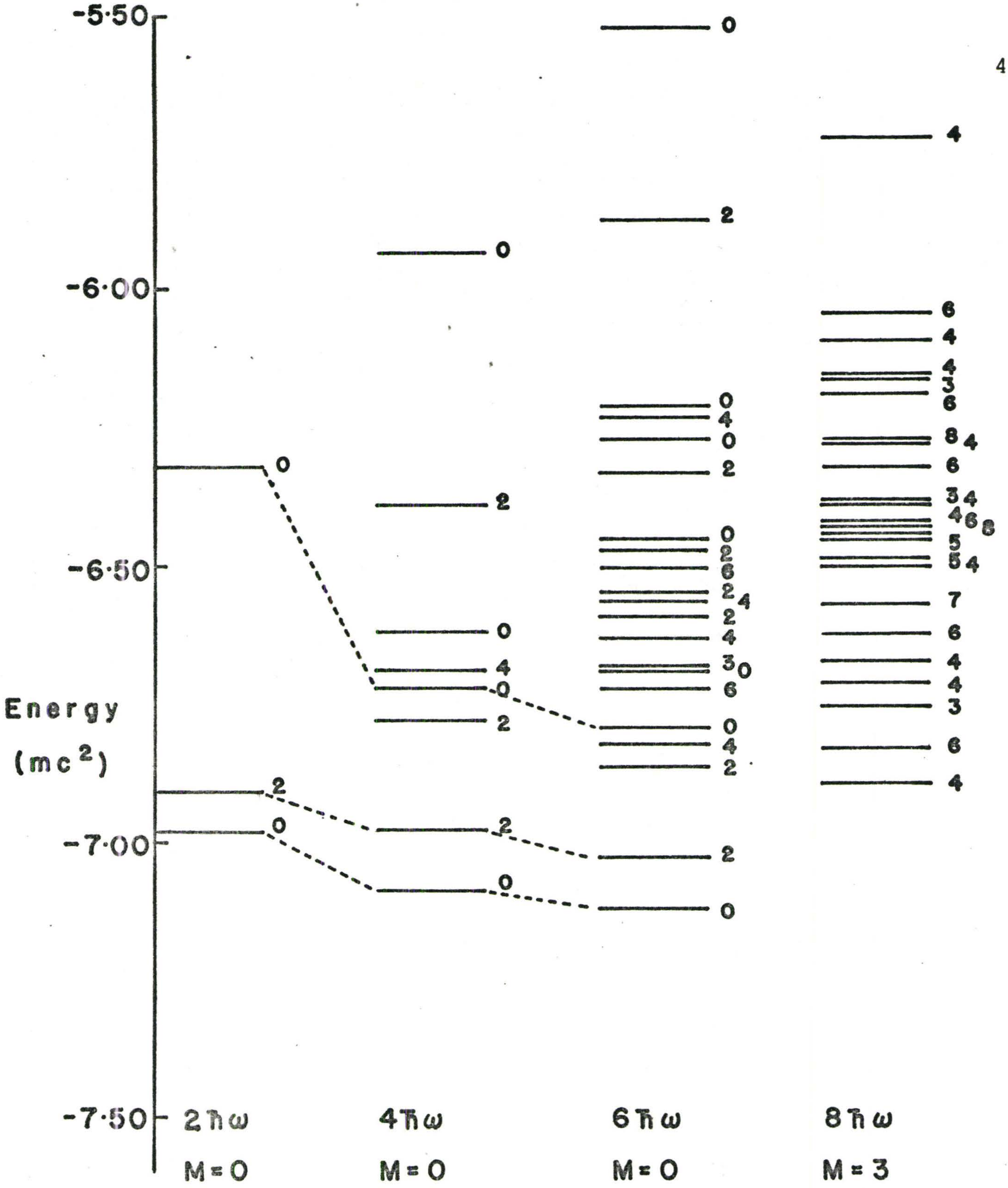


FIGURE 15 - ENERGY LEVELS FOR POTENTIAL I

from calculations using each basis for potentials I and III; the highest excitation possible was $8\hbar\omega$, with M=3 (matrix size 231). The dotted lines connect a few corresponding states resulting from the use of different bases. Note that the energies in these figures are expressed in units of mc^2, not μc^2. Clearly the levels generated using potential I (soft) change much less when the basis is increased than do the levels generated by potential III. This is to be expected, since the more extreme (i.e. rapidly changing with r) the potential, the more basis states are needed to construct a good wavefunction.

In spite of the failure to obtain accurate eigenstates, a certain amount of information can still be gleaned from the results. If the B(E2)'s for transitions between the states are calculated, we find that it is possible to separate the states into bands, as in the two-particle case, for which the B(E2)'s for in-band transitions are greater than those for cross-band transitions. Although the values of the B(E2)'s change by as much as 10% as the basis is increased, the ratios of the B(E2)'s change only by a maximum of about 4%; thus, we can be sure that this separation of states into bands is indeed correct. Fig. 16 shows the three lowest bands for states generated using potential I. A few representative B(E2)'s are also shown in this figure. The maximum number of states of a given J in a band is seen to be $\frac{J}{2} + 1$ for J

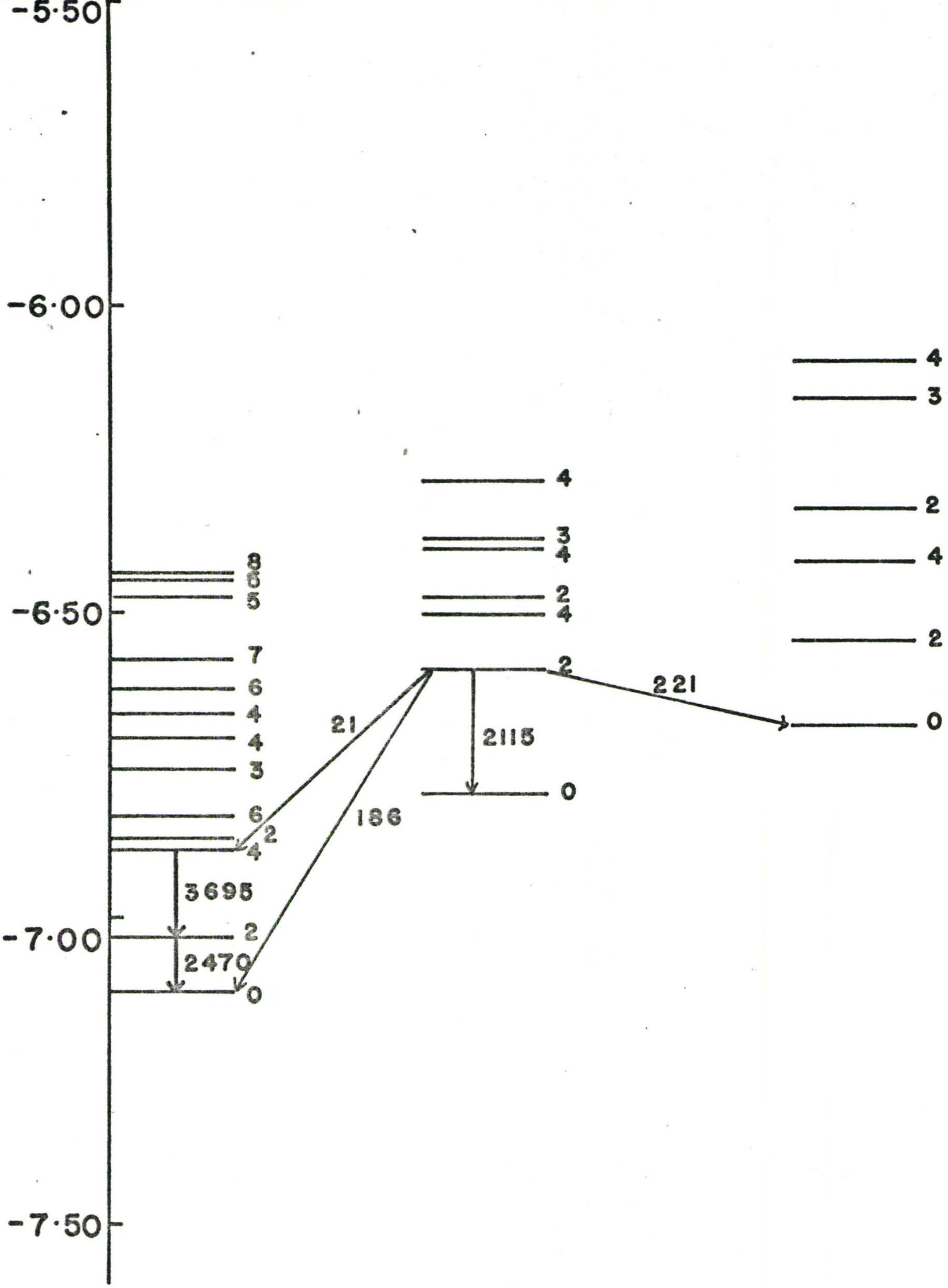


FIGURE 16 - ROTATIONAL-VIBRATIONAL BANDS

(POTENTIAL I)

even, and $\frac{J-1}{2}$ for J odd. This corresponds exactly with the number of states of a given J for a rigid asymmetric rotor, with wavefunctions which transform according to the A representation (totally symmetric) of the D_2 group (Appendix C). In demanding that our wavefunctions be symmetric with respect to particle interchange, we have restricted our wavefunctions to transform according to the A representation of the D_2 group.

One of the surprising features of the calculation was the number of centre of mass excited states which were produced. For the $8\hbar\omega$, M=3 case, in which there were a total of 231 states, 207 of these were centre of mass excitations and thus were useless for our purposes.

Discussion and Conclusions

The qualitative reproduction of many experimental observations by our naive two-particle model of the nucleus is rather interesting. It seems to indicate that a rough picture of a rotating and vibrating axially symmetric nucleus can be gotten by considering each end of the nucleus to be a boson, and letting these bosons interact via a two-body potential. Assuming that this model is qualitatively valid, we see then that the nucleus stretches as its vibrational and rotational energies increase. As well, even though a nucleus does not display a strict J(J+1) energy dependence, it still may be classified as rotational.

The three-particle results were disappointing. Although we managed to obtain distinct rotational bands, we had hoped to investigate deviations from the energy relations for a rigid asymmetric rotor (i.e. the sum of the energies of all states of a given even J equals the sum of the energies of all states of angular momentum (J+1)) as a function of the potential used. Clearly the next step that could be taken in this problem would be to construct basis states of definite J (see Table I). It would then be possible to form a basis consisting of all excitations of no more than $10\hbar\omega$ above the basis ground state. This size of basis would probably be enough to give accurate eigenstates, at least for the softer potentials.

APPENDIX A

EVALUATION OF INTEGRALS $R_{qs}^{(\pm n)}$ AND $Z_{qs}^{(\pm n)}$

(a) $\underline{R_{qs}^{(\pm n)}}$

$$R_{qs}^{(+n)} = \int_0^\infty P_{n_q m_q}(\sqrt{\alpha_q}\ \rho)\rho^n P_{n_s m_s}(\sqrt{\alpha_s}\ \rho)\rho d\rho \quad .$$

For generality, it has been assumed here that the oscillator constants in the states q and s may be different. Then,

$$R_{qs}^{(+n)} = 2\sqrt{\frac{\alpha_q\ \alpha_s\ n_q!\ n_s!}{(n_q+|m_q|)!\ (n_s+|m_s|)!}}\ \alpha_q^{\frac{1}{2}|m_q|}\ \alpha_s^{\frac{1}{2}|m_s|}\int_0^\infty \rho^{n+1+|m_q|+|m_s|}$$

$$\times\ L_{n_q}^{|m_q|}(\alpha_q\ \rho^2)\ L_{n_s}^{|m_s|}(\alpha_s\ \rho^2)\ e^{-\frac{1}{2}(\alpha_q+\alpha_s)\rho^2}\ d\rho \quad .$$

Now

$$L_n^m(\alpha\rho^2) = \sum_{u=0}^{n}\frac{(n+m)!\ (-\alpha)^u\ \rho^{2u}}{(n-u)!\ (m+u)!\ u!} \qquad \text{(I-7)}$$

$$R_{q_s}^{(+n)} = 2\sqrt{\alpha_q\ \alpha_s\ n_q!\ n_s!\ (n_q+|m_q|)!\ (n_s+|m_s|)!}\ \alpha_q^{\frac{1}{2}|m_q|}\ \alpha_s^{\frac{1}{2}|m_s|}$$

$$\times \sum_{u=0}^{n_q}\sum_{v=0}^{n_s}\frac{(-1)^{u+v}\ \alpha_q^u\ \alpha_s^v}{(n_q-u)!\ (|m_q|+u)!\ u!\ (n_s-v)!\ (|m_s|+v)!\ v!}$$

$$\times \int_0^\infty \rho^{n+1+|m_q|+|m_s|+2u+2v}\ e^{-\frac{1}{2}(\alpha_q+\alpha_s)\rho^2}\ d\rho \qquad .(1)$$

It is easy to show that:

$$\int_0^\infty \rho^{\ell} e^{-b\rho^2} d\rho = (\frac{1}{2b})^{\frac{\ell+1}{2}} \; 2.4.6\ldots(\ell-1) \quad \text{for } \ell \text{ odd}$$

$$= \frac{1.3.5\ldots(\ell-1)}{2^{\frac{\ell}{2}} \, . \, b^{\frac{\ell}{2}}} \sqrt{\frac{\pi}{b}} \quad \text{for } \ell \text{ even} \qquad .(2)$$

Using (2) and (1) with $\ell = n+1+ m_q + m_s +2u+2v$, and $b = \frac{1}{2}(\alpha_q+\alpha_s)$, $R_{ij}^{(+n)}$ is then determined. $R_{ij}^{(+n)}$ can be obtained simply by replacing the α's in the above with their inverses.

(b) $\underline{Z_{qs}^{(\pm n)}}$

$$Z_{qs}^{(+n)} = \int_{-\infty}^{\infty} Z_{n_{z_q}}(\sqrt{a_q}\; z)\; z^n \; Z_{n_{z_s}}(\sqrt{a_s}\; z)dz \qquad ,$$

where it has been assumed that a_q and a_s may be different.

Now

$$Z_{qs}^{(+n)} = (\frac{a_q a_s}{\pi^2})^{1/4} \sqrt{\frac{1}{2^{n_{z_q}+n_{z_s}} \, . \, n_{z_q}! \, . \, n_{z_s}!}} \int_{-\infty}^{\infty} H_{n_{z_q}}(\sqrt{a_q}\; z) z^n$$

$$\times H_{n_{z_s}}(\sqrt{a_s}\; z)\; e^{-\frac{1}{2}(a_q+a_s)z^2} dz \qquad .$$

From Lebedev$^{(12)}$,

$$H_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k \; n!}{k! \; (n-2k)!} (2x)^{n-2k} \qquad ,$$

where $[\nu]$ denotes the largest integer $\leqslant \nu$.

Thus,

$$z_{qs}^{(+n)} = \left(\frac{a_q a_s}{\pi^2}\right)^{1/4} \sqrt{\frac{1}{2^{n_{z_q}+n_{z_s}} \cdot n_{z_q}! \cdot n_{z_s}!}} \, (2\sqrt{a_q})^{n_{z_q}} (2\sqrt{a_s})^{n_{z_s}}$$

$$\times \sum_{k=0}^{[n_{z_q}/2]} \sum_{\ell=0}^{[n_{z_s}/2]} \frac{(-1)^{k+\ell} (2\sqrt{a_q})^{-2k} (2\sqrt{a_s})^{-2\ell}}{k!\ \ell!\ (n_{z_q}-2k)!\ (n_{z_s}-2\ell)!}$$

$$\times \int_{-\infty}^{\infty} z^{n_{z_q}+n_{z_s}+n-2k-2\ell} \, e^{-\frac{1}{2}(a_q+a_s)z^2} \, dz \quad .$$

If $(n_{z_q}+n_{z_s}+n)$ is odd, the integral in the last line is trivially zero. If $(n_{z_q}+n_{z_s}+n)$ is even, the integral may be rewritten as:

$$2 \int_{0}^{\infty} z^{n_{z_q}+n_{z_s}+n-2k-2\ell} \, e^{-\frac{1}{2}(a_q+a_s)z^2} \, dz$$

and evaluated by Eq. (2). Thus $z_{qs}^{(+n)}$ is determined; $z_{ij}^{(-n)}$ can be gotten by replacing the a's with their inverses.

APPENDIX B

POTENTIAL MATRIX ELEMENTS$^{(11)}$

The matrix elements we want to evaluate are $\langle qr|V'_{12}|st\rangle$. Since V'_{12} is the sum of an attractive and a repulsive Gaussian, we consider a general matrix element of the form $\langle qr|e^{-\frac{1}{2}K(\underline{r}_1-\underline{r}_2)^2}|st\rangle$, where the factor of ½ appears in the exponential merely to correspond to Copley's and Volkov's notation. The matrix element may be broken up into two parts, the radial and angular part M and the z-part I. The final expression for the radial and angular part is:

$$M = C\, 2^{|m_q|+|m_s|+2}\, \pi^2\, \alpha_q^{\frac{1}{2}|m_q|}\, \alpha_r^{\frac{1}{2}|m_r|}\, \alpha_s^{\frac{1}{2}|m_s|}\, \alpha_t^{\frac{1}{2}|m_t|}\, K^{|m_s-m_q|}$$

$$\times\ \lambda^{\frac{1}{2}(|m_r|+|m_t|-|m_q|-|m_s|)}\quad k^{-(|m_s-m_q|+|m_r|+|m_t|+2)}$$

$$\times \sum_{u=0}^{n_q}\ \sum_{v=0}^{n_r}\ \sum_{v=0}^{n_s}\ \sum_{x=0}^{n_t}\ \sum_{y=0}^{n}\ n!\ (\tfrac{1}{2}(|m_s-m_q|+|m_r|+|m_z|)+v+x+y)!$$

$$\times\, \mathcal{L}_{n_q u}^{|m_q|}\left(\frac{4\alpha_q}{\lambda}\right)\, \mathcal{L}_{n_r v}^{|m_r|}\left(\frac{\alpha_r\lambda}{k^2}\right) \mathcal{L}_{n_s w}^{|m_s|}\left(\frac{4\alpha_s}{\lambda}\right)\, \mathcal{L}_{n_t x}^{|m_s|}\left(\frac{\alpha_t\lambda}{k^2}\right)$$

$$\times\, \mathcal{L}_{ny}^{|m_s-m_q|}\left(-\,\frac{K^2}{k^2}\right) \tag{1}$$

$$\text{where } C = \frac{1}{\pi^2}\sqrt{\frac{\alpha_q\ \alpha_r\ \alpha_s\ \alpha_t\ n_q!\ n_r!\ n_s!\ n_t!}{(n_q+|m_q|)!\ (n_r+|m_r|)!\ (n_s+|m_s|)!\ (n_t+|m_t|)!}}\ ,$$

$$\lambda = 2(\alpha_q+\alpha_s+K) ,$$

$$k^2 = (\alpha_r+\alpha_t)(\alpha_q+\alpha_s) + K(\alpha_q+\alpha_r+\alpha_s+\alpha_t) ,$$

$$2n = |m_q|+|m_s|-|m_s-m_q|+2u+2w ,$$

and $$\mathscr{L}^{m}_{pf}(\chi) = \frac{(p+m)!\ (-\chi)^f}{(p-f)!\ (m+f)!\ f!} .$$

Although 5 sums are involved in Eq. (1), the number of terms involved in any given sum is quite small, and the sums can be evaluated quite easily by machine computation. It should be noted that for the sake of generality it has been assumed that the α's may be different in each state; this adds only one summation to (1) however.

The z-part of the matrix element is:

$$I = D\,\frac{2\pi}{k} \sum_{u=0}^{[n_s]} \sum_{v=0}^{[\min(n_q,n_s-2u)]} \sum_{w=0}^{[n_q+n_s-2u-2v]} \sum_{x=0}^{[n_r]} \sum_{y=0}^{[n_t]} 2^{v+n}\ v!$$

$$\times \binom{n_q}{v} \binom{n_s-2u}{v} \frac{(n_q+n_s-2u-2v-2w)!\ (n_r-2x)!\ (n_t-2y)!}{(n-n_q-n_s+2u+2v+2w)!\ (n-n_r+2x)!\ (n-n_t+2y)!}$$

$$\times \left(\frac{a_s-a_q+K}{a_q+a_s+K}\right)^{\frac{1}{2}(n_q+n_s-2u-2v)} h_{n_s u}\left(\left(\frac{a_s}{a_q}\right)\right)^{\frac{1}{2}}$$

$$\times h_{(n_q+n_s-2u-2v)w}\left(\left(\frac{2a_q\ K^2}{(a_s-a_q+K)k^2}\right)\right)^{\frac{1}{2}} h_{n_r x}\left(\left(\frac{4a_r}{k^2}\right)\right)^{\frac{1}{2}}$$

$$\times h_{n_t y}\left(\left(\frac{4a_t}{k^2}\right)\right)^{\frac{1}{2}} \qquad (2)$$

where $$D = \frac{1}{\pi^2}\sqrt{\frac{(a_q a_r a_s a_t)^{\frac{1}{2}}}{2^{(n_q+n_r+n_s+n_t)}\ n_q!\ n_r!\ n_s!\ n_t!}} ,$$

$$k^2 = (a_q+a_s)(a_r+a_t) + K(a_q+a_r+a_s+a_t) ,$$

$[\nu]$ denotes the largest integer $\leqslant\nu$,

$\min(n_1,n_2)$ denotes the lesser of n_1 and n_2 ,

$\binom{n_1}{n_2}$ is the binomial coefficient ,

$$2n = n_q+n_r+n_s+n_t-2u-2v-2w-2x-2y ,$$

$$h_{mP}(\chi) = \frac{m!\ \chi^{m-2P}\ (\chi^2-1)^P}{P!\ (m-2P)!} ,$$

and $$\lambda = \tfrac{1}{2}(a_q+a_s+K) .$$

Note in the above that n_z has been replaced everywhere by n, in order to uncomplicate the indices slightly. For the expression (2) to be non-vanishing, $(n_q+n_r+n_s+n_t)$ must be an even number (otherwise 2n would be odd).

The matrix element $\langle qr|e^{-\frac{1}{2}K(\underline{r}_1-\underline{r}_2)^2}|st\rangle$ is then obtained by the product of M and I.

APPENDIX C

RIGID ROTORS AND THE D_2 GROUP(18,20)

Consider a rigid object with body-fixed axes X,Y,Z, whose orientation with respect to the laboratory axes X,Y,Z is determined by the Euler angles α,β,γ. The rotational Hamiltonian for such an object is:

$$H = \tfrac{1}{2}\left[\frac{T_X^{\,2}}{I_X} + \frac{T_Y^{\,2}}{I_Y} + \frac{T_Z^{\,2}}{I_Z}\right] \qquad ,(1)$$

where I_X, I_Y, I_Z are the principal moments of inertia along the X,Y,Z axes respectively (we assume the X,Y,Z axes to coincide with the principal axes of the body), and T_X, T_Y, T_Z are the components of the angular momentum $\hat{T}$ of the body (an equivalent way of looking at $\hat{T}$ is to say that it generates an infinitesimal rotation of the body). T_X, T_Y, T_Z operate on the Euler angles α,β,γ and satisfy the commutation relations:

$$[T_X,T_Y] = -i\hbar\, T_Z \quad \text{(and cyclic permutations)} \qquad .$$

Note that since $\hat{T}$ rotates the body, instead of the coordinate system, the commutation relations differ by a minus sign from the usual angular momentum commutation relations.

Also,

$$T^2 \; D^J_{MK}(\alpha\beta\gamma) = \hbar^2 \; J(J+1) \; D^J_{MK}(\alpha\beta\gamma)$$

$$T_Z \; D^J_{MK}(\alpha\beta\gamma) = \hbar \; K \; D^J_{MK}(\alpha\beta\gamma)$$

$$T_Z \; D^J_{MK}(\alpha\beta\gamma) = \hbar \; M \; D^J_{MK}(\alpha\beta\gamma)$$

where the D's are the generalized spherical functions. Write

$$a = \frac{1}{I_X} \; , \; b = \frac{1}{I_Y} \; , \; c = \frac{1}{I_Z} \quad .$$

Then
$$H = \tfrac{1}{2}(aT_X{}^2 + bT_Y{}^2 + cT_Z{}^2) \quad .(2)$$

If all three moments of inertia of the body are different ($a \neq b \neq c$, $a \neq c$) then the body is an asymmetric rotor. Eigenfunctions ψ^J of H corresponding to angular momentum J can be written as linear combinations of D functions ϕ_{JK} (M is irrelevant for our purposes).

$$\psi_J = \sum_K g_K \; \phi_{JK} \quad (3)$$

where

$$\phi_{JK} = \sqrt{\frac{2J+1}{8\pi^2}} \; D^J_{MK}(\alpha\beta\gamma) \quad .$$

Hence for a given J-value, we construct the Hamiltonian matrix elements $<\phi_{JK}|H|\phi_{JK'}>$, and diagonalize to obtain the eigenvalues of H. For each J, the Hamiltonian matrix is

(2J+1) x (2J+1) in size. We can simplify the problem and reduce the sizes of the matrices to be diagonalized by considering the symmetry properties of H. We may then classify the rotational states with respect to the irreducible representations of the appropriate symmetry group and diagonalize in each irreducible representation, since the matrix elements of H between wavefunctions belonging to different irreducible representations of the appropriate group are zero.

H is invariant under the operations of the D_2 symmetry group. This group contains the identity element and 3 rotations by Π about the 3 axes X,Y,Z. The character Table of the D_2 group is written below:

D_2	E	C_X^2	C_Y^2	C_Z^2
A	1	1	1	1
B_1	1	-1	-1	1
B_2	1	-1	1	-1
B_3	1	1	-1	-1

TABLE IV

CHARACTER TABLE OF THE D_2 GROUP

We want to consider wavefunctions which transform according to the A representation, i.e. linear combinations of the ϕ_{JK} which transform according to the A representation. Clearly $N(E+C_X^{\ 2}+C_Y^{\ 2}+C_Z^{\ 2})D^J_{MK} = \psi_A^{JK}$ is a function which transforms according to the A representation (N is a normalization constant), since

$$E\ \psi_A^{JK} = \psi_A^{JK}$$

$$C_X^{\ 2}\ \psi_A^{JK} = \psi_A^{JK},\ \text{etc.} \qquad .$$

Operating with the C's above, using the expressions for $C_X^{\ 2}\ D^J_{MK}$, etc., from Davydov$^{(20)}$, we get

$$\psi_A^{JK} = N[1+(-1)^K]\ [D^J_{MK}+(-1)^J\ D^J_{M,-K}] \qquad .(4)$$

Note that only even values of K are allowed, and if K=0, J must be even; as well, ψ_A^{JK} is symmetric in K and (-K). For J=0, there is only one state (K=0); for J=1, there are no states, etc. If J is even, there are $\frac{J}{2}+1$ states, and for J odd, there are $\frac{J-1}{2}$ states. For a given J-value, we may now construct matrix elements of H between wavefunctions of the form (4) and diagonalize, thus giving the eigenvalues in the A-representation. It may be shown that the sum of the energies of all states of a given even J equals the sum of the energies of all states of angular momentum (J+1).

REFERENCES

(1) T. A. Brody and M. Moshinsky, Tables of Transformation Brackets (Gordon and Breach, 1967) p. xlvii

(2) A. Erdelyi et al, Higher Transcendental Functions, Vol. 2 (McGraw-Hill, 1953) p. 188

(3) ibid, p. 190

(4) A. Erdelyi et al, Tables of Integral Transforms, Vol. 1 (McGraw-Hill, 1954) p. 175

(5) ibid, p. 373

(6) M. A. Preston, Physics of the Nucleus (Addison-Wesley, 1962) p. 299

(7) ibid, p. 614

(8) M. E. Rose, Elementary Theory of Angular Momentum (John Wiley, 1957) p. 62

(9) M. R. D. P. Manning, Ph.D. Thesis (McMaster University, 1967) p. 168

(10) ibid, p. 172

(11) L. A. Copley and A. B. Volkov, Nucl. Phys. <u>84</u> (1966) 417

(12) N. N. Lebedev, Special Functions and Their Applications (Prentice-Hall, 1965) p. 60

(13) G. Herzberg, Spectra of Diatomic Molecules (Van Nostrand, 1950)

(14) J. O. Newton et al, Nucl. Phys. <u>A141</u> (1970) 631

(15) R. A. Gough, Ph.D. Thesis (McMaster University, 1970)

(16) G. Herzberg, Infrared and Raman Spectra (Van Nostrand, 1945)

(17) ibid, p. 50

(18) J. P. Davidson, Collective Models of the Nucleus (Academic Press, 1968) p. 33

(19) C. N. Banwell, Fundamentals of Molecular Spectroscopy (McGraw-Hill, 1966) p. 69

(20) A. S. Davydov, Quantum Mechanics (Pergamon Press, 1965) p. 472