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Oliver Davis Johns
(Ph.D. Thesis)

November 1968

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UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
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Oliver Davis Johns
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Pairing in Nuclei

Abstract

Oliver Davis Johns

Parts I and II of this thesis deal with the general problem of adapting the quasi-particle approximation to give satisfactory results in nuclear systems. Part I shows that the projection of correct particle number from the number non-conserving quasi-particle ground state vector can give excellent agreement with exact ground states, when the quasi-particle ground state is first modified by an exponential four, eight, etc., quasi-particle operator.

The similarity of this ground state exponential form to that predicted by the quasi-boson method leads to Part II, which considers the generalized problem of computing both ground and excited seniority zero 0+ states of nuclei. The results of Part II demonstrate that excellent overlap of boson and exact 0+ states is obtained if the following revisions are made in the quasi-boson method:

(1) The zero energy boson used to help define the boson ground state should be a certain linear sum of the spurion and its conjugate, and not the spurion alone.

(2) The first excited state for moderate to weak pairing potential strength is a two boson state consisting of one zero energy boson and one non-zero energy boson.

(3) The striking failure of the method at subshell closures can be circumvented by slightly altering the average particle number.

Part III of the thesis illustrates the method of exact, number conserving diagonalization of the many body Hamiltonian matrix. This method, which is practical only for non-deformed nuclear systems, is conceptually simpler than the quasi-particle method in which much effort must go into the isolation and correction of approximation produced inaccuracies.

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GENERAL INTRODUCTION

In 1958, it was suggested that the energy gap in the spectra of even-even nuclei could be predicted by using approximation methods from the theory of superconductivity to treat a phenomenological nuclear pairing force[1]). A pairing force in nuclei is here taken to be an attractive two body force acting most strongly between states of time reversed pairs of identical particles. (This thesis will consider only pairing of like particles, although many results presented here are also relevant to n-p pairing.)

This initial suggestion was pursued by others[2,3]). Impressive qualitative agreement with nuclear spectra, moments of inertia, etc., was obtained. However, as the calculations were refined, doubts arose as to the accuracy of the methods being used. First, the state vectors from the superconductivity approximation are not eigenstates of particle number. An approximate ground state of the Ni^{60} neutron system, for example, contains large components with 28, 30, 34, and 36 neutrons, as well as the desired 32. Second, the approximation fails at closed subshells when the pairing potential strength is reduced below a certain value. Both of these problems reflect the difference between a system of some 10^{22} electrons per cubic centimeter in a metal lattice and a system of some hundred nucleons in a nucleus.

This thesis is a study of methods of dealing with

pairing forces in nuclei. It is divided into three parts. In Part I, the quasi-particle formalism developed in the theory of superconductivity is outlined, and methods of adapting the formalism briefly discussed. Part I concludes with a numerical investigation of what is, in a certain sense, the maximum accuracy obtainable from the quasi-particle approximation with projection of exact particle number. It can be considered a feasibility study leading to Part II, which is a theoretical and numerical study of the quasi-boson or linearization method applied to the nuclear pairing force problem. Part II concludes that if certain precautions and limitations are observed, the method can predict well the ground and first excited seniority zero, 0+ states of nuclear systems. Part III is a departure from I and II in the it abandons the quasi-particle approximation in favor of exact diagonalization of pairing potentials, in seniority truncated spaces. A method is developed which allows, for example, exact diagonalization of single closed shell nuclear systems far from shell closures. The utility of this method, which is similar to the quasi-spin formalism, is that the complexity and time cost of the computation are not much greater than those of some of the more elaborate methods based on the quasi-particle approximation. The results, however, are exact within the space comsidered. The method is illustrated by application to several single closed shell nuclei.

References

1) A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev., 110 (1958) 936

2) S. T. Belyaev, Mat. Fys. Medd. Dan. Vid. Selsk., 31, No. 11 (1959)

3) L. S. Kisslinger and R. A. Sorensen, Mat. Fys. Medd. Dan. Vid. Selsk,, 32, No. 9 (1960)

PART I

PROJECTION METHODS

1. Brief Introduction to Nuclear Pairing

Most research into nuclear spectra is presently based on the shell model[1]), in which individual nucleons are assumed to move independently in a single particle potential which is presumed to represent their average mutual attraction. Techniques such as the Hartree-Fock method exist which can, in principle at least, extract an effective single particle potential from a known two body potential acting among many nucleons[2]). However, at the present time most calculations of nuclear spectra take the assumed single particle energies either directly from experimental observation or from a phenomenological single particle potential well based on experimental observation, or from a combination of both.

It is found that the correct prediction of the energy levels, transition rates, etc., of nuclear spectra also requires the assumption of a residual two body potential in addition to the above single particle one[3]). Thus the model of an actual nuclear system has state vectors which are superpositions of the various configurations (arrangements) of nucleons among the single particle levels.

In the many body formalism, the Hamiltonian of nucleons in single particle orbits with configurations mixed by a two body residual potential, V, is

$$H = \sum_{\alpha} e_{\alpha} c_{\alpha}^{+} c_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \bar{v} | \gamma\delta \rangle c_{\alpha}^{+} c_{\beta}^{+} c_{\delta} c_{\gamma} \qquad (1)$$

The operator $c_\alpha^+ c_\alpha$ counts the number of particles in the state labeled by α, and c_α^+ and c_α create and annihilate a particle, respectively, in the same state. The e_α is the single particle energy of the state. The bar over V indicates that the two body matrix element is taken between anti-symmetric two body states. Since nucleons are fermions,

$$\{c_\alpha, c_\beta^+\} = c_\alpha c_\beta^+ + c_\beta^+ c_\alpha = \delta_{\alpha\beta} \tag{2}$$

The exact form of the states labeled by the subscripts depends on the transformation properties assumed for H, as well as the scheme chosen for coupling the particles in many particle states. For this thesis, most use will be made of systems in which H is assumed invariant under rotations and in which each single particle state is taken as a state of definite total (spin plus orbital) angular momentum. This is the j-j coupling model, in which subscript α stands for n_α, ℓ_α, j_α, m_α; where n_α is the number of radial nodes, ℓ_α is the orbital angular momentum, j_α the total angular momentum, and m_α is the "z" component of total angular momentum of the single particle wave function. The subscript could also indicate that the particle is a neutron or a proton. However, for the present purposes this is not necessary, since only like nucleon mixing will be treated.

By a simple and well known algebraic identity, H can be

rewritten, for any potential, V, in the form

$$H = \sum_j e_j n_j + \frac{1}{4} \sum_{\substack{i'j'ij \\ J}} \bar{G}(i'j'ijJ) \sum_M a^+_{i'j'}(JM)\, a_{ij}(JM) \tag{3}$$

where

$$\bar{G}(i'j'ijJ) = \langle (i'j')JM | v | (ij)JM \rangle + (-1)^{i-j+J} \langle (i'j')JM | v | (ji)JM \rangle$$

$$|(ij)JM\rangle = \sum_{qm} |iqjm\rangle \langle iqjm|JM\rangle \quad .$$

$$n_j = \sum_m c^+_{jm} c_{jm}$$

and

$$a^+_{ij}(JM) = \sum_{qm} \langle iqjm|JM\rangle\, c^+_{iq}\, c^+_{jm} \quad . \tag{4}$$

The $\langle iqjm|JM\rangle$ are vector coupling coefficients. We have followed the usual practice of labeling state n,l,j,m simply by j,m (or i,q). The identity follows from the definitions by direct substitution, using the known symmetries of the vector coupling coefficients. The integer J is the total angular momentum of a pair of particles and M is its "z" component.

A pure pairing potential is one for which

$$\bar{G}(i'j'ijJ) = 0 \qquad \text{for} \quad J \neq 0 \quad . \tag{5}$$

Then

$$H = \sum_j e_j n_j - \sum_{ij} G_{ij} \, \Omega_i^{1/2} \, \Omega_j^{1/2} \, a_i^+ a_j \tag{6}$$

where

$$G_{ij} = - \frac{\bar{G}(iijj0)}{\sqrt{(2i+1)}\sqrt{(2j+1)}}$$

$$\Omega_j = \frac{1}{2}(2j+1)$$

and

$$a_j^+ = \frac{1}{\sqrt{2}} a_{jj}^+(00) \quad . \tag{7}$$

In the m-basis, H for a pure pairing potential is

$$H = \sum_{jm} e_j c_{jm}^+ c_{jm} - \sum_{\substack{ij \\ q,m>0}} G_{ij} \, c_{iq}^+ (-1)^{i-q} c_{i-q}^+ (-1)^{j-m} c_{j-m} \, c_{jm} \quad . \tag{8}$$

A constant, pure pairing potential has $G_{ij} = G$, a constant, for all i,j. This latter has been much used as a phenomenological potential of extreme simplicity, which is nonetheless capable of introducing configuration mixtures known to exist in nuclear systems.

It is obvious that any potential, V, has a pure pairing potential as its J = 0 term. Moreover, for short range potentials, such as the delta function potential, the terms with J = 0 are systematically smaller that the J = 0 term.

2. The Quasi-particle Approximation

Assume a pure pairing potential (as in eq. (6)) acting among n nucleons in some single particle basis. First, assume n to be even. It follws simply from the commutation relations of a_j^+ and n_j (see Part III of this thesis) that the exact spectrum of seniority zero (all pairs coupled to J = 0), 0+ states of the system, including the ground state, can be obtained by diagonalizing H in the space created by various products of the different a_j^+ operators. However, the dimension of the space may be impractically large in some cases. For example, for 2p particles in 2p levels each with $j = \frac{1}{2}$, there are $\binom{2p}{p}$ configurations. For p = 10, a fairly small number for actual calculations in the deformed region, $\binom{20}{10}$ is greater than 10^5. For such cases, a simplified state vector is obviously necessary. The one discussed here was first introduced in the theory of superconductivity[4]). The formalism, which is well known, will be outlined here for reference.

Instead of the exact form

$$\sum_{pq\cdots} C_{pq\cdots} \, (a_i^+)^p \, (a_j^+)^q \cdots |0\rangle \tag{9}$$

where the sum is over all configurations satisfying p + q + ... = n/2, an approximate ground state vector

$$|\tilde{0}\rangle = \prod_j \left[\sum_{p=0}^{\Omega_j} U_j^{\Omega_j - p} V_j^p \binom{\Omega_j}{p}^{\frac{1}{2}} \eta_j^{-1}(p) \, (a_j^+)^p \right] |0\rangle \tag{10}$$

is used, where

$$\eta_j^2(p) = \langle 0 | (a_j)^p (a_j^+)^p | 0 \rangle$$

is a normalization factor, and U_j, V_j are real and positive. In the m-basis,

$$|\tilde{0}\rangle = \prod_{\substack{j \\ m>0}} \left(U_j + V_j \, c_{jm}^+ (-1)^{j-m} c_{j-m} \right) |0\rangle \tag{11}$$

The vector $|\tilde{0}\rangle$ is called the quasi-particle vacuum state. Normalization requires $U_j^2 + V_j^2 = 1$. Thus the approximate ground state vector has, instead of the large number of coefficients, $C_{pq\ldots}$, only one independent paramenter, V_j, per single particle level.

Particle number conservation is violated by $|\tilde{0}\rangle$. The average particle number is set equal to the correct value,

$$n = \langle \tilde{0} | \bar{n} | \tilde{0} \rangle = \sum_j 2 V_j^2 \Omega_j \tag{12}$$

where

$$\bar{n} = \sum_j n_j \quad .$$

One can proceed to minimize the expectation value of H, subject to the constraint (12),

$$\delta \langle \tilde{0} | H - \lambda \bar{n} | \tilde{0} \rangle = 0 \quad . \tag{13}$$

The Lagrange multiplier, λ , is then the Fermi energy of the system,

$$\lambda = \frac{d}{dn} \langle \tilde{0} | H | \tilde{0} \rangle \quad . \tag{14}$$

An equivalent procedure[5]) is to make a canonical transformation from operators c^{+}_{jm} to operators α^{+}_{jm} defined by

$$\alpha_{jm} | \tilde{0} \rangle = 0 \quad . \tag{15}$$

It follows that

$$\alpha^{+}_{jm} = U_j \, c^{+}_{jm} - V_j \, (-1)^{j-m} \, c_{j-m} \quad . \tag{16}$$

Then $H - \lambda \bar{n}$, with H from eq. (6), is rewritten in terms of α^{+}_{jm} and α_{jm} , and the V_j parameters are chosen to diagonalize $H - \lambda \bar{n}$, except for terms containing products of four of the new operators. This reduces $H - \lambda \bar{n}$ to the form

$$H - \lambda \bar{n} = H_0 + \sum_{jm} E_j \, \alpha^{+}_{jm} \alpha_{jm} \tag{17}$$

$$+ \text{ terms with four operators} ,$$

where term H_0 contains no operators. The result is

$$V_j^2 = \frac{1}{2}\left(1 - \frac{e_j - \lambda}{E_j}\right) \tag{18}$$

with

$$E_j = \left[(e_j - \lambda)^2 + \Delta_j^2 \right]^{\frac{1}{2}} \tag{19}$$

and

$$\Delta_i = \sum_j G_{ij} U_j V_j \Omega_j \tag{20}$$

leading to the consistency condition

$$\Delta_i = \frac{1}{2} \sum_j G_{ij} \frac{\Delta_j \Omega_j}{E_j} \tag{21}$$

Also,

$$n = \sum_j 2 V_j^2 \Omega_j \tag{22}$$

The approximate ground state of an even system is then $|\tilde{0}\rangle$, and the approximate excited states are of the form

$$\alpha_{iq}^{+} \alpha_{jm}^{+} |\tilde{0}\rangle$$

The approximate ground state energy is $H_0 + \lambda n$. The excited states are thus separated in energy from the ground state by at least $(\Delta_i + \Delta_j)$, which is of the order of 1 MeV. They are separated from each other by $(E_{i'} + E_{j'} - E_i - E_j)$ which is of the order of KeV. This reproduces a striking regularity of the spectra of even-even nuclei. The ground state of an odd system is

$$\alpha^+_{jm} |\tilde{0}\rangle$$

and there is no energy gap between the odd ground and excited states. The operator α^+_{jm} is a superposition of a particle operator and a hole operator; it is called a quasi-particle creation operator. The quasi-particle α^+_{jm} creates an elementary excitation of energy E_j, which is called the quasi-particle energy.

3. Projection of Exact Particle Number

Two immediate shortcomings of the quasi-particle approximation just outlined are: (1) number non-conservation, and (2) the vanishing of non-trivial solutions for some values of parameters (weak pairing).

(1). The ground state vector, eq. (10), is a product of sums. Each sum has p of the a_j^+ operators in its pth term, with p running from 0 to Ω_j. Hence the product, when the factors are multiplied out, contains terms with every even number of particles from 0 to 2Ω, where Ω is the sum of all Ω_j. That is,

$$|\tilde{0}\rangle = \sum_{p=0}^{\Omega} z_p \, |\Gamma_p\rangle \tag{23}$$

where $|\Gamma_p\rangle$ denotes all those terms from $|\tilde{0}\rangle$ which obey

$$\bar{n} \, |\Gamma_p\rangle = 2p \, |\Gamma_p\rangle \quad . \tag{24}$$

(The operator n counts the total number of particles in all levels.) In realistic calculations, the distribution of $|z_p|^2$ versus p is peaked about the correct average value determined by eq. (12). The rms spread of this distribution may amount to some 10 or 12 particles. Thus the quasi-particle approximation results in the averaging of any calculated properties over a set of neighboring nuclei. In

its unmodified form, it should not be expected to distinguish those properties which vary sharply from one nucleus to the next.

(2). When the average particle number, n, is equal to a closed subshell of particles, the consistency equation (21) has only the trivial solution $\Delta_j = 0$ whenever the potential strength, G_{ij}, is less than a certain critical value, G_c[6]). (Set $G_{ij} = GX_{ij}$ and then decrease G. For $G < G_c$, the only solution is $\Delta_j = 0$.) When $\Delta_j = 0$, eqs. (18) show that

$$V_j^2 = 1 \quad \text{when} \quad e_j < \lambda \,,$$
$$V_j^2 = 0 \quad \text{when} \quad e_j > \lambda \,. \tag{25}$$

Since λ moves to a point between the last filled subshell and the first empty one, the result is a state $|\tilde{0}\rangle$ with only the one configuration giving the least single particle energy. This can be seen by substituting eqs. (25) into eq. (10). This vanishing of configuration mixture for non-zero values of G_{ij} is a failure of the approximation method. It is not found in the exact solution to the problem.

A number of methods[13]) designed to deal with failure (2) have been proposed. The methods retain the number non-conservation implicit in eqs. (10), (11) but modify eqs. (18) - (22). We will concentrate here on a method for overcoming failures (1) and (2) by, essentially, abandoning eqs. (18) - (22), and

retaining only the form of $|\tilde{0}\rangle$ and the definition of a quasi-particle, α^{+}_{jm}. (See eqs. (10), (11), and (16).)

Consider a projection operator Z_k, defined by

$$Z_k = \prod_{\substack{t=0 \\ t\neq k}}^{2\Omega} \left(\frac{\bar{n}-t}{k-t}\right) . \tag{26}$$

Then

$$Z_{k=2p}\,|\tilde{0}\rangle = z_p\,|\Gamma_p\rangle ,$$

$$Z_{k=2p}\,|\Gamma_p\rangle = |\Gamma_p\rangle , \tag{27}$$

$$\bar{n}\, Z_{k=2p}\,|\tilde{0}\rangle = 2p\, Z_{k=2p}\,|\tilde{0}\rangle .$$

This operator picks out of $|\tilde{0}\rangle$ those terms having k particles. It is found[7]) that if, in a nuclear system, one solves the quasi-particle equations (18) - (22) for an average n, and then operates on the ground state vector by Z_n, the quantity

$$\mathcal{E}_n = \frac{\langle\tilde{0}|\, Z_n H Z_n\,|\tilde{0}\rangle}{\langle\tilde{0}|\, Z_n\,|\tilde{0}\rangle} \tag{28}$$

is closer to the exactly calculated ground state energy for the system than is the term $H_0 + \lambda n$ in eq. (17). Also, of course, the resulting eigen function

$$|\Phi\rangle = \mathcal{N} Z_n |\tilde{0}\rangle \,, \tag{29}$$

where $\mathcal{N}$ is a normalization factor, is an exact eigen state of particle number. In ref.[7]), the authors also projected correct particle number from the seniority one states, $\alpha^{+}_{jm}|\tilde{0}\rangle$, of odd isotopes of Ni and found, after normalization, better than 0.99 overlap with state vectors from an exact matrix diagonalization. However, since eqs. (18) - (22) were first solved for the V_j, before Z_n was applied, failure (2), above, still is present.

Other workers[8]) abandoned eqs. (18) - (22) entirely, and instead developed a formalism to minimize the energy directly as a function of variational parameters V_j^2. Using a saddle point method, they prove that the minimum point in V_j^2 space is always non-trivial for an attractive potential. Configuration mixing is present for all non-zero values of G_{ij}.

A later paper[9]) performed calculations using a delta potential in deformed nuclei, using both the method of projecting after using eqs. (18) - (22), which the authors call PBCS, and the method of ref.[8]), which they call FBCS. (PBCS and FBCS stand respectively for projected or fixed particle treatment of the superconductivity state vector first proposed by Bardeen, Cooper and Schrieffer.) The paper[9]) finds that,

as predicted, the FBCS method always leads to non-trivial solutions, and further, that it always predicts more configuration mixing than the PBCS method. The authors find that in regions of strong configuration mixing (large G_{ij}), the FBCS and PBCS methods give similar results. This similarity for large G_{ij} is interesting when one considers that the region of Ni isotopes treated in ref.[7]) by the PBCS method, is a region of particularly strong mixing. The question of the overlap of PBCS or FBCS state vectors with exact state vectors is left unresolved for the case when G_{ij} is small.

A comparison has been made[10]) of the exact and PBCS state vectors for a simple model system of two $j = 9/2$ levels containing 10 particles. The authors of this study find that for large force strength ($G_{ij} = G$ assumed constant), the exact and approximate state vectors are very close, a result similar to that obtained for the Ni isotopes[7]). Of course, since the system[10]) has a closed subshell, eqs. (18) - (22) give only a trivial solution for small G, and the PBCS method fails there.

For small G values in a similar model system, another paper[11]) reports that the FBCS method, although it gives non-trivial solutions for small G values, tends to underestimate the amount of configuration mixing, compared to exact solutions. The authors found that this underestimation could be somewhat corrected by introducing a four quasi-particle term into the ground state. The results of this paper will be discussed in detail, and extended, in the next section.

4. A Two Parameter Approximation

Consider a model system of two single particle levels of equal total angular momentum, j, and containing (2j + 1) particles. Each level can contain up to $\Omega_j = \frac{1}{2}(2j+1)$ pairs of particles. The system is thus half full. The symmetry of this system simplifies the theoretical treatment of it. However, it is complex enough to show features of actual nuclear systems. Consider the Hamiltonian, eq. (6), acting in this system, with constant $G_{ij} = G$,

$$H = \sum_r e_r n_r - G \sum_{r,s} \sqrt{\Omega_r}\sqrt{\Omega_s}\, a_r^+ a_s \qquad (30)$$

Since both levels have the same j value, we have changed notation slightly to denote levels by integer subscripts. When $g = G/(e_2 - e_1) << 1$, the correct ground state vector for this system can be written, to leading order in g

$$|\Phi\rangle = \sum_q^{\Omega_1} C_q \,|\Omega_1 - q \quad q\rangle \qquad (31)$$

with

$$C_q = q! \binom{\Omega_1}{q} \left(\tfrac{1}{2} g\right)^q$$

and

$$|p\ q\rangle = \mathcal{N}_1^{-1}(p)\, \mathcal{N}_2^{-1}(q)\, (a_1^+)^p\, (a_2^+)^q\, |0\rangle$$

where the $\mathcal{N}$'s are normalizing factors as before. This result follows from eq. (30) by the use of perturbation theory, keeping the leading order term for each C_q.

The quasi-particle approximate ground state vector for this same system is (eq. (6))

$$|\tilde{0}\rangle = \sum_{p=0}^{\Omega_1} \sum_{q=0}^{\Omega_2} U_1^{\Omega_1-p} V_1^{p} \binom{\Omega_1}{p}^{\frac{1}{2}} U_2^{\Omega_2-q} V_2^{q} \binom{\Omega_2}{q}^{\frac{1}{2}} |p\ q\rangle . \quad (32)$$

Operating with Z_k, where $k = 2\Omega_1$, gives terms with $p+q=\Omega_1$,

$$Z_{2\Omega_1}|\tilde{0}\rangle = \sum_{q=0}^{\Omega_1} U_1^{q} V_1^{\Omega_1-q} U_2^{\Omega_1-q} V_2^{q} \binom{\Omega_1}{q} |\Omega_1-q\ \ q\rangle \quad (33)$$

which can be rewritten in terms of a single free parameter, X.

$$X = \frac{U_1 V_2}{V_1 U_2} = \left(\frac{V_2}{V_1}\right)^2 \quad (34)$$

(No generality is lost by taking $U_1 = V_2$ and hence $V_1 = U_2$.)

$$Z_{2\Omega_1}|\tilde{0}\rangle = \sum_{q=0}^{\Omega_1} \binom{\Omega_1}{q} X^q |\Omega_1-q\ \ q\rangle \quad (35)$$

(Note that eq. (35) is normalized to unity only in the limit X = 0.)

For this system, the eqs. (18) - (22) have a solution in closed form, due to the symmetry of the half filled system. Since the number of particles is just sufficient to fill the

lower subshell, there is a critical value of G

$$G_c = \frac{e_2 - e_1}{\Omega_2 + \Omega_1} \tag{36}$$

such that $G < G_c$ implies $\Delta = 0$. (Since Δ_j is a constant when G_{ij} are all equal, the subscript on Δ_j is suppressed here.) Therefore, for small values of G, we cannot expect the PBCS method to give good results. It will give simply the trivial solution. That is,

$$Z_{2\Omega_1} |\tilde{0}\rangle = |\Omega_1 \; 0\rangle \tag{37}$$

when

$$G < G_c$$

The form of eq. (35) shows that the FBCS method for this system reduces simply to minimizing eq. (28) with $n = 2\Omega_1$,

$$\mathcal{E}_{2\Omega_1}(X) = \frac{\langle\tilde{0}| Z_{2\Omega_1} H Z_{2\Omega_1} |\tilde{0}\rangle}{\langle\tilde{0}| Z_{2\Omega_1} |\tilde{0}\rangle} \tag{38}$$

as a function of the single free parameter, X. Before performing this minimization, it is, therefore, reasonable to ask if there is any value of X, no matter how arrived at, which will reproduce the perturbation result of eq. (31) in the $g \ll 1$ limit. Thus, we want to know if any value of X

satisfies (eq. (31) and eq. (35))

$$C_q = \binom{\Omega_1}{q} X^q \qquad q = 0, 1, 2, \ldots \tag{39}$$

where

$$C_q = q! \binom{\Omega_1}{q} \left(\tfrac{1}{2} g\right)^q \quad .$$

It is obvious that the terms C_0 and C_1 can be matched to leading order in g if we set

$$X = \frac{1}{2} g \quad . \tag{40}$$

But then the right hand side of eq. (39), which is the FBCS result, will be smaller than C_q by a factor of q! for all values of q. The minimization procedure based on the state vector of eq. (35) is inadequate to reproduce the coefficients of q pairs promoted from the lower level to the upper level, whenever q is greater than one.

Ref.[11]) noted that agreement between the coefficient C_2 and the FBCS result could be improved by introducing a four quasi-particle term into the trial function, eq. (35), giving

$$Z_{2\Omega_1} \left(1 + \beta A_1^+ A_2^+\right) |\tilde{0}\rangle \tag{41}$$

where

$$A_j^+ = \frac{1}{\sqrt{2}} \sum_m \langle j\, m\, j{-m} | 00 \rangle\, \alpha_{jm}^+ \alpha_{j-m}^+ \tag{42}$$

and where β is a new variational parameter to be chosen. They noted that β and X could be chosen to improve the agreement with C_2 while retaining the already exact (to leading order) correspondence with coefficients C_0 and C_1.

This result suggests the following more general one[12]. The operators A_j^+, which create a normalized pair of quasi-particles coupled to zero angular momentum, are related to the operators a_j^+ by

$$A_j^+ = U_j^2 a_j^+ - V_j^2 a_j + \sqrt{\Omega_j}\, U_j V_j \left(1 - \frac{n_j}{\Omega_j}\right) \tag{43}$$

as can be seen by substituting eq. (16) into eq. (42) directly, and using the commutation relations and definitions above. Then, if X = 0, it follows that

$$A_1^+ \longrightarrow -a_1$$

$$A_2^+ \longrightarrow a_2^+$$

and therefore that

$$Z_{2\Omega_1} e^{\beta A_1^+ A_2^+} |\tilde{0}\rangle \longrightarrow \sum_{q=0}^{\Omega_1} q! \binom{\Omega_1}{q} \left(\frac{-\beta}{\Omega_1}\right)^q |\Omega_1 - q \;\; q\rangle \tag{44}$$

where only leading order terms for each q have been retained. Comparison with eq. (31) shows that if the choice

$$X = 0$$
$$\beta = -\frac{1}{2}\Omega_1 g \tag{45}$$

is made, the state vector

$$Z_{2\Omega_1} e^{\beta A_1^+ A_2^+} |\tilde{0}\rangle \tag{46}$$

reproduces correctly the coefficients C_q to leading order for all values of q from zero to Ω_1 .

This small G result complements the success of the PBCS method for large G, and suggests that a superior approximate ground state vector can be obtained if one generalizes the FBCS method to a minimization of

$$\mathcal{E}_{2\Omega_1}(\beta, x) = \frac{\langle\tilde{0}| e^{\beta A_2 A_1} Z_{2\Omega_1} H Z_{2\Omega_1} e^{\beta A_1^+ A_2^+} |\tilde{0}\rangle}{\langle\tilde{0}| e^{\beta A_2 A_1} Z_{2\Omega_1} e^{\beta A_1^+ A_2^+} |\tilde{0}\rangle} \tag{47}$$

as a function of the two parameters, β and X, for all values of G. One expects that as G becomes large, the β parameter will become vanishingly small and the state vector, eq. (46), will go over to the form found to be correct in the large G limit.

The energy function, eq. (47), was calculated for general β and X, for a system of two levels with equal j = 9/2 and (2j + 1) = 10 particles. The minimum point in the β,

X plane was found for g values between 0.01 and 1.0, using an electronic computer. (The value of $(e_2 - e_1)$ is taken as unity, so there is no distinction needed between g and G below.) Figures 1 and 2 show contour maps of $\mathcal{E}_{2a_1}(\beta, X)$ for two different values of G. It is seen that in each case a minimum exists for a small negative value of β. Three coefficient ratios C_q/C_0 are shown in Figures 3, 4, and 5 for three different computational methods. The exact result (calculated by methods described in Part III of this thesis) is shown as a solid line. The one parameter minimization result, using eq. (38), is labeled FBCS. The two parameter result, using eq. (47), is labeled Exponential FBCS. One sees that the Exponential FBCS gives good agreement with the ratios over the whole range of G values. The FBCS method, however, underestimates the higher ratios badly. For example, C_3/C_0 is underestimated by a factor of 2 at G = 0.1, which is the critical value, G_c, for the parameters used. Since realistic nuclear calculations often involve force strengths just above critical, this underestimation could have a serious effect on the calculated values of physical quantities, such as E0 transition rates. Figure 6 shows the minimum energy values of β and X for various values of G. It is seen that β does become small for large G, as anticipated above.

Thus a two parameter minimization correctly reproduces five coefficient ratios C_q/C_0 over a range of G values from

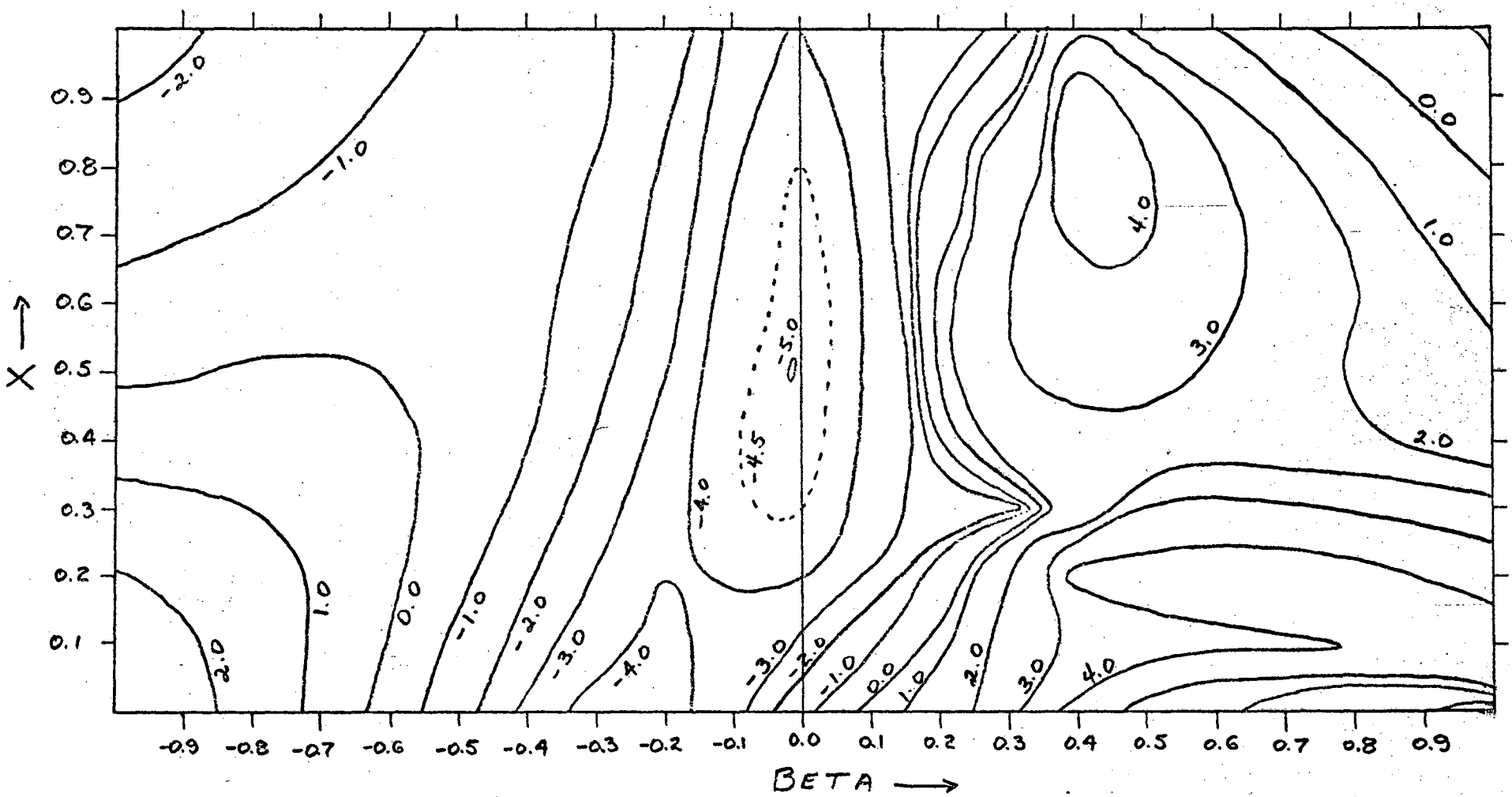


Fig. 1. Contour plot of $\mathcal{E}_{2\Omega_1}(\beta, X)$, eq. (47), versus β and X. The parameters are $g = 0.3$, $\Omega_1 = \Omega_2 = 5$, and $(e_2 - e_1) = 1.0$ MeV. Contour heights are in MeV.

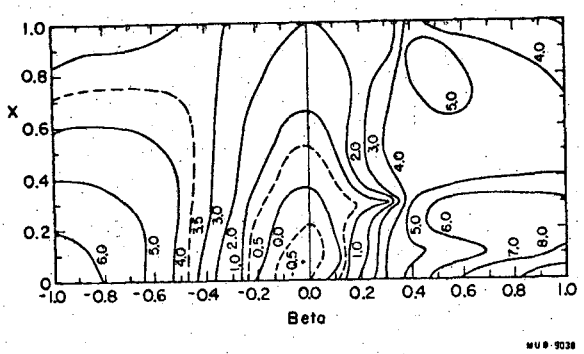


Fig. 2.

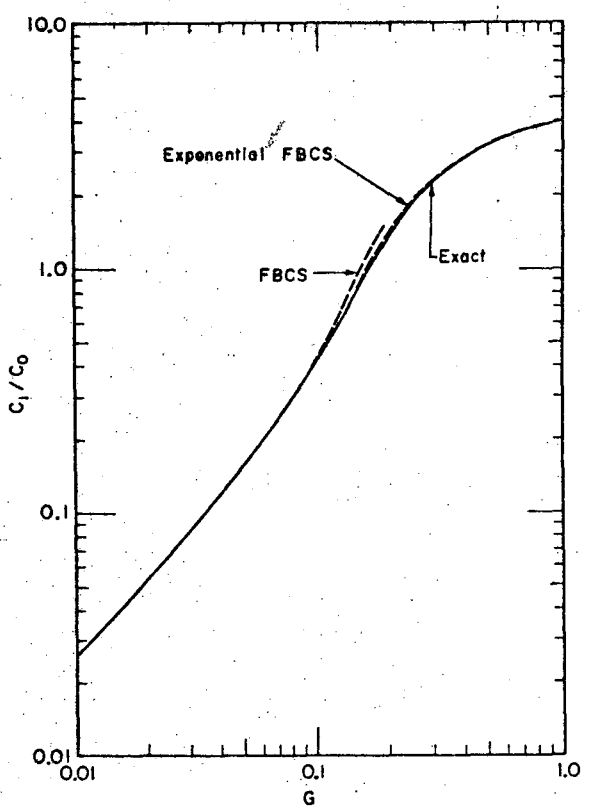
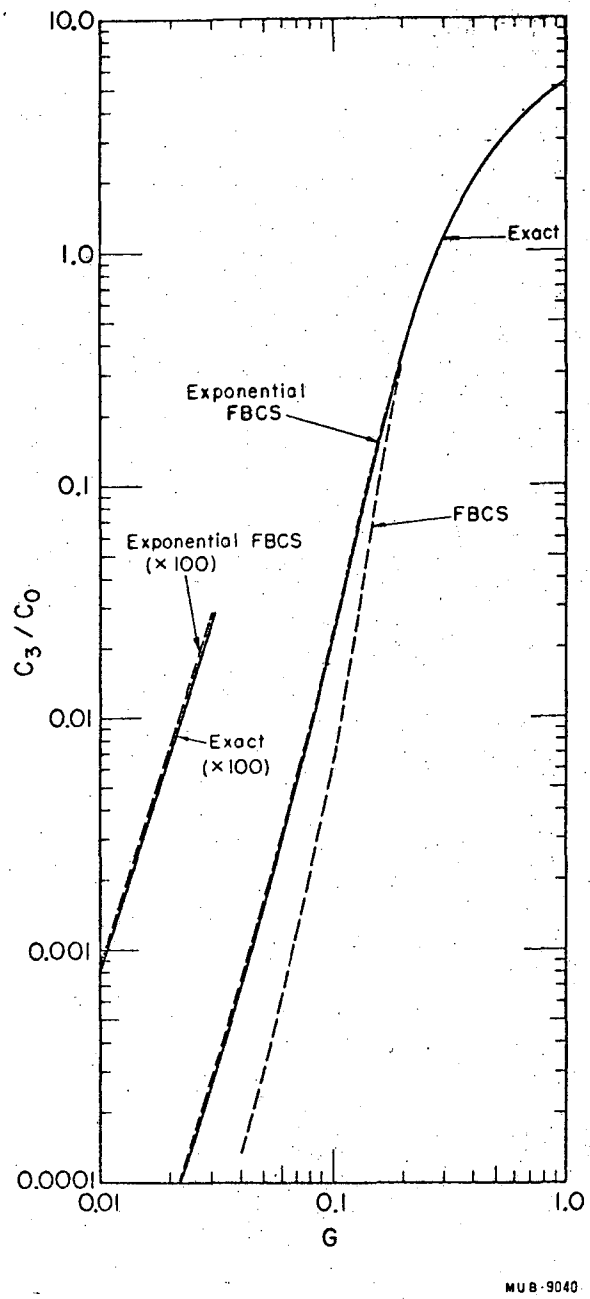


Fig. 3.

Fig. 2. Contour plot of $\mathcal{E}_{2\Omega_1}(\beta, X)$, eq. (47), versus β and X. The parameters are g = 0.1, $\Omega_1 = \Omega_2 = 5$, and $(e_2 - e_1) = 1.0$ MeV. Contour heights are in MeV.

Fig. 3. The coefficient ratio C_1/C_0 for one pair promoted to the upper level is compared for exact, FBCS (eq. 38), and exponential FBCS (eq. 47) ground states. The G values are in MeV. The $(e_2 - e_1) = 1.0$ MeV.



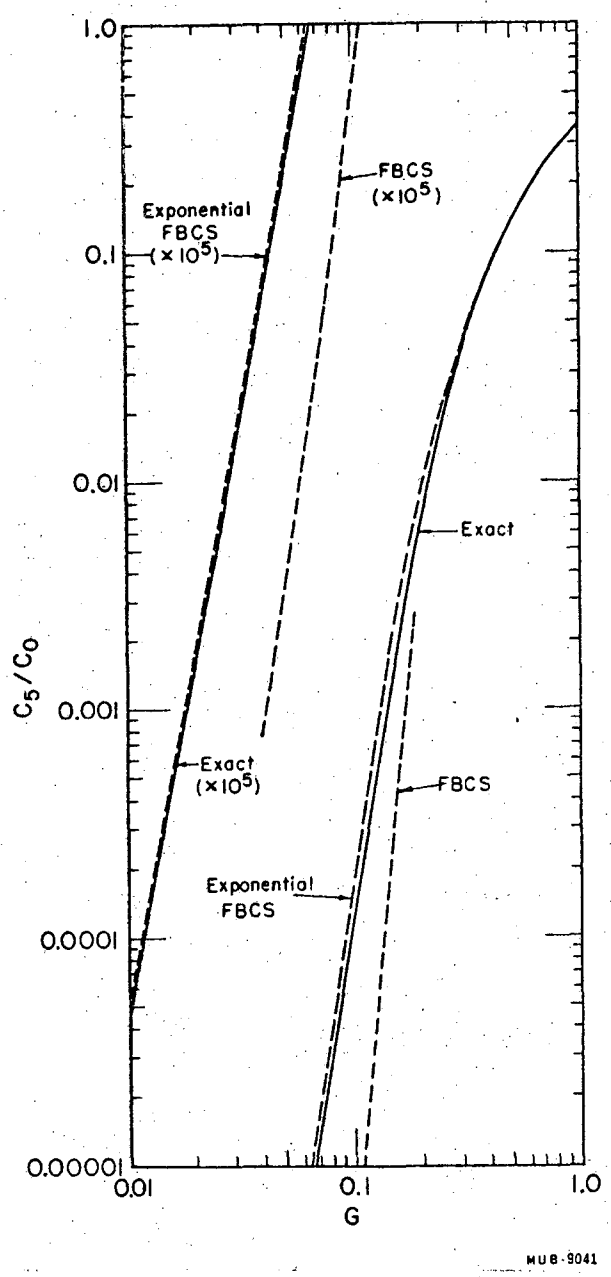


Fig. 4

Fig. 5

Fig. 4. The coefficient ratio C_3/C_0 for three pairs promoted to the upper level is compared as in Fig. 3.

Fig. 5. The coefficient ratio C_5/C_0 for five pairs promoted to the upper level is compared as in Fig. 3.

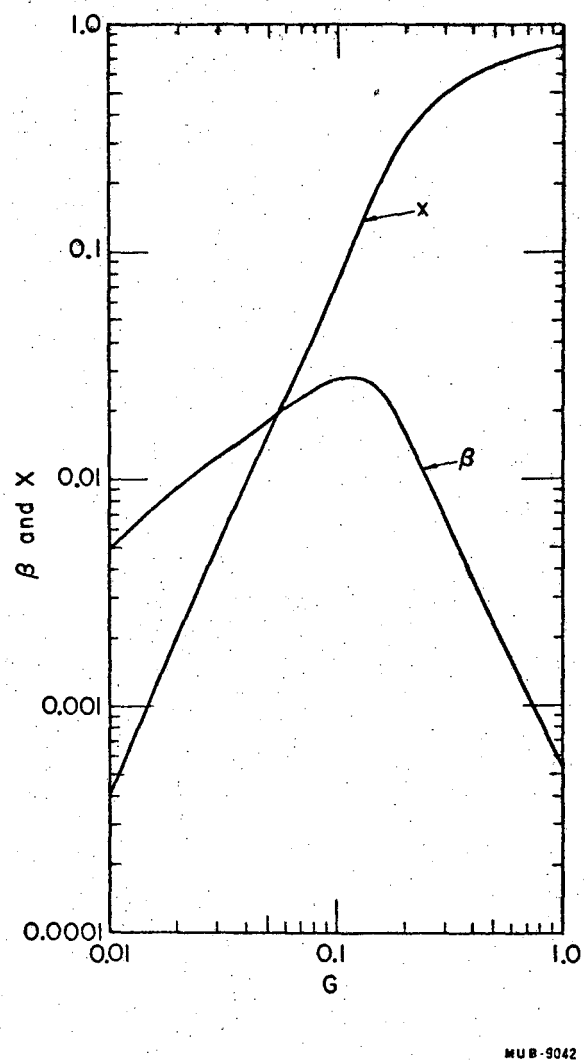


Fig. 6. Values of β and X giving minimum values for $\mathcal{E}_{2\Omega_1}(\beta, X)$, eq. (47). The G values are in MeV. Parameters are $\Omega_1 = \Omega_2 = 5$, $(e_2 - e_1) = 1.0$ MeV.

0.01 to 1.0. It would appear that, while the two parameter fixed particle number variational form, eq (46), will not significantly lower the variational energy below the FBCS method, eq. (35), nonetheless the smaller amplitudes in the state vector may be greatly improved over FBCS in the range of pairing force strength encountered in calculations of real nuclear systems.

5. Possible Generalizations

The approximate ground state vector in eq. (46) was arrived at above by comparison with perturbation theory in a particular model system. A similar form of ground state vector is predicted by the quasi-boson approximation applied to the pairing problem. It is

$$|gnd\rangle = K\, e^{\frac{1}{2}\sum_{ij}\beta_{ij} A_i^{+} A_j^{+}}\, |\tilde{o}\rangle \tag{48}$$

where β_{ij} is a symmetric matrix, and K is a normalization factor. (The quasi-boson method is discussed extensively in Part II of this thesis, so result will only be quoted here.) When the quasi-boson method is applied to the symmetric model system above, β_{ij} becomes a 2x2 matrix with zero diagonal terms, which is exactly the form of eq. (46) if we put $\beta_{ij} = \beta_{ji} = \beta$. It would therefore seem reasonable to generalize by projecting correct particle number from eq. (48) and using it as a variational form. However, it is shown in Part II that the PBCS method (solving the quasi-particle equations, eqs. (18) - (22), and then projecting correct particle number) can be extended by the quasi-boson technique to give good state vectors for ground and lowlying seniority zero, 0+ excited states. The critical behavior (trivial solution below $G = G_c$) problem is largely overcome in Part II by setting the particle number at a slightly incorrect value,

away from a closed subshell. The quasi-boson, PBCS method of using the quasi-particle and quasi-boson equations followed by number projection can be applied to any system, and has the advantage of also predicting lowlying excited states with good accuracy. Because of this success, and because of the complications which arise in the quasi-boson formalism when eqs. (18) - (22) are invalid, the combining of FBCS and quasi-boson methods is not pursued further here.

6. Conclusions

The results of Part I, then, can be considered as a test, in a model system, to determine the maximum accuracy which can be expected from ground state vectors of the form predicted by the quasi-boson method. The quasi-boson method, of course, makes definite predictions of the values of β and X for each value of G, but the numerical results just presented do not use those predictions. The results obtained show that in the system considered, very good accuracy in the reproduction of ground state vectors is possible using trial vectors of the project quasi-boson exponential form. Failure of the quasi-boson method to give good ground state vectors in some regions is therefore probably due to errors in the method of predicting the parameters equivalent to β and X, and not to the exponential form of the ground state used.

References to Part I

1) M. G. Mayer and J. H. D. Jensen, Elementary Theory of Nuclear Shell Structure (John Wiley and Sons, New York, 1955)

2) G. E. Brown, Unified Theory of Nuclear Models (North Holland, Amsterdam, 1964) p. 11.

3) J. P. Elliot and A. M. Lane, Handbuch der Physik XXXlX (Springer, Berlin, 1957) p. 241.

) A. de Shalit and I. Talmi, Nuclear Shell Theory (Academic Press, New York, 1963)

4) Bardeen, Cooper, and Schrieffer, Phys. Rev. 108 (1957) 1175

5) N. N. Bogolubov, Nuovo Cimento 7 (1958) 794
J. G. Valatin, Nuovo Cimento 7 (1958) 843

6) S. T. Belyaev, Mat. Fys. Mett. Dan. Vid. Selsk. 31, No. 11 (1959)

7) A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. 124 (1961) 162

8) K. Dietrich, H. J. Many, and J. Pradal, Phys. Rev. 135 (1964) B22

9) H. J. Mang, J. K. Poggenburg, and J. O. Rasmussen, Nuc. Phys. 64 (1965) 353

10) M. Rho and J. O. Rasmussen, Phys. Rev. 135 (1964) B1295

11) H. J. Mang, J. O. Rasmussen, and M. Rho, Phys. Rev. 141 (1966) 941

12) O. Johns and J. O. Rasmussen, A New Particle-Conserving Variational Wave Function for the Nuclear Pairing-Force Problem, Nuclear Chemistry Division Annual Report, UCRL 16580 (1965) 29

13) V. G. Solov'ev, Doklady Akad. Nauk. SSSR 133 (1960) 325. Translation: Soviet Physics Doklady 5 (1961) 778
Y. Nogami, Phys. Rev. 134 (1964) B313

PART II

THE QUASI-BOSON METHOD

1. Introduction

This is a theoretical and numerical study of the quasi-boson approximation to the 0+ spectrum of spherical nuclei, and to β-vibrations in deformed nuclei.

In sections 2 and 3 the quasi-boson formalism is derived. These sections, included for completeness and reference, are similar to previously-published developments[1]).

Section 4 discusses the zero-energy boson solution which is characteristic of the theory. Two ideas are developed which contrast with previous publications:

(1) The correct zero-energy boson is not the spurion state alone (denoted $Q^{(0)+}$ in eq. (25)) but a certain linear combination of it and its conjugate boson.

(2) The zero-energy boson is not always deserving of the name "spurious", but rather, for medium to low force strength becomes a legitimate part of the excitation spectrum - filling a gap in the spectrum that would otherwise exist.

Section 5 shows how the zero-energy-bosons are related to number fluctuation states. A criterion is given fixing the particular linear combination of $Q^{(0)+}$ and its conjugate to be used in (1), above. Also, a primitive pair vibration is postulated which connects quasi-particle vacuum states of slightly different force strength.

Section 6 shows how an essential failure of the quasi-particle method can be circumvented.

Section 7 applies the theory above to a simple model system consisting of two $j = 9/2$ levels. Cases are considered with various force strengths and with eight and ten particles (closed subshell). The predictions of the quasi-boson method are compared directly with the exact states of various energy and particle number.

Although the numerical work uses a constant pairing force, the formalism presented is applicable also to non-constant pairing forces. The formulas are presented for the case of spherical nuclei (j a good quantum number). However, this restriction is in no way essential. The results, in very similar form, apply also to deformed nuclei.

The main conclusion of the paper is that the quasi-boson-approximation may be useful for many systems applicable to real nuclei, but that the methods must be used with care. Particular attention must be paid to the different choices of boson forms to be used for weak and strong pairing force strengths, and to circumventing the failure of the method at closed shells or subshells when the pairing-force is moderate to weak in strength.

2. The Quasi-Boson Approximation

The Hamiltonian, H, for a system of identical nucleons in spherical j-j coupling shell model orbitals, with configuration mixed by two-body potential, V, is

$$H = \sum_{j\nu} e_j c^{+}_{j\nu} c_{j\nu} + \frac{1}{2} \sum_{\substack{ij i'j' \\ \sigma\nu\sigma'\nu'}} \langle i'\sigma' j'\nu' | V | i\sigma j\nu \rangle c^{+}_{i\sigma'} c^{+}_{j'\nu'} c_{j\nu} c_{i\sigma} .$$

The indices i, j, i', j' run over the (half-integral) angular momentum quantum numbers of the various orbitals. The index, j, thus stands for the full set of quantum numbers necessary to specify the orbital. The indices, ν, σ, are the "z" components of angular momentum for the orbits j and i respectively. The operators $c^{+}_{j\nu}$ and $c_{j\nu}$ create and annihilate a fermion in orbit $j\nu$. The e_j is the relative shell-model energy of orbital j.

The Hamiltonian, H, can be written in an equivalent form

$$H = \sum_{j\nu} e_j c^{+}_{j\nu} c_{j\nu} + \frac{1}{4} \sum_{\substack{ij i'j' \\ J}} \bar{G}(i'j'ijJ) \sum_{M} a^{+}_{i'j'}(JM)\, a_{ij}(JM)$$

where

$$\bar{G}(i'j'ijJ) = \langle (i'j')JM | V | (ij)JM \rangle + (-1)^{i-j+J} \langle (i'j')JM | V | (ji)JM \rangle ,$$

$$| (ij)JM \rangle = \sum_{\nu\sigma} | i\sigma j\nu \rangle \langle i\sigma j\nu | ijJM \rangle ,$$

and

$$a^{+}_{ij}(JM) = \sum_{\nu\sigma} \langle i\sigma j\nu | ijJM \rangle\, c^{+}_{i\sigma} c^{+}_{j\nu} . \qquad (1)$$

The total angular momentum of a pair, J, takes integer values. The "z" component of the total angular momentum of a pair, M, takes integer values from -J to +J. Note that $\bar{G}(i'j'ij\ J)$ does not depend on M.

If the values $\bar{G}(i'j'ij\ J)$ obey

$$\left|\bar{G}(i'j'ij\,J)\right| \ll \left|\bar{G}(j'j'jj\,0)\right|$$

for all J > 0 and all i', j', i, j, and if V is attractive, then the potential, V, is said to be a generalized pairing potential[2]). The only effect of $\bar{G}(i'j'ij\ J)$ for J > 0 on the quasi-boson 0+ spectrum comes through self-energy corrections to the e_j. These corrections may be included, if desired, by replacing each e_j by

$$e_j + \sum_{J>0} \frac{(2J+1)}{(2j+1)} \sum_i \bar{G}(ij\,ij\,J)\, V_i^2$$

in the following (except that the correction should be multiplied by 1/2 in the case of H_0, eq. (6)).

The quasi-boson formalism has previously[1]) been derived with the approximation of constant pairing potential

$$(2i+1)^{-\frac{1}{2}}\,(2j+1)^{-\frac{1}{2}}\,\bar{G}(iijj\,0) = -G$$

where G is a constant energy.

The derivation outlined here will be for the slightly more general (but not completely general) case in which the pairing potential can be approximated

$$(2i+1)^{-\frac{1}{2}}\,(2j+1)^{-\frac{1}{2}}\,\bar{G}(iijj0) = -G\,\chi_i\,\chi_j \quad .$$

With this approximation, the part of Hamiltonian relevant to the quasi-boson 0+ spectrum becomes

$$H = \sum_j e_j n_j - G \sum_{ij} \chi_i \chi_j \Omega_i^{\frac{1}{2}} \Omega_j^{\frac{1}{2}} a_i^+ a_j \tag{2}$$

where

$$\begin{aligned} n_j &= \sum_\nu c_{j\nu}^+ c_{j\nu} \,, \\ \Omega_j &= (j + \tfrac{1}{2}) \,, \\ a_j^+ &= 2^{-\frac{1}{2}} a_{jj}^+(00) \,. \end{aligned} \tag{3}$$

The Hamiltonian is now re-written in terms of quasi-particles

$$\alpha_{j\nu}^+ = U_j\, c_{j\nu}^+ - V_j\,(-1)^{j-\nu}\, c_{j\,-\nu}$$

with the parameters U_j, V_j defined by the usual equations[2])

$$\begin{aligned} \begin{bmatrix} U_j^2 \\ V_j^2 \end{bmatrix} &= \frac{1}{2}\left(1 \pm \frac{e_j - \lambda}{E_j}\right) , \\ E_j &= \left[(e_j - \lambda)^2 + \Delta_j^2\right]^{\frac{1}{2}} , \\ \Delta_i &= G\chi_i \sum_j \chi_j \Omega_j U_j V_j \,, \\ 2/G &= \sum_j \chi_j^2 \Omega_j E_j^{-1} \quad \text{when} \quad \bar{\Delta} = \frac{\Delta_j}{\chi_j} \neq 0 \,, \\ n &= \sum_j 2V_j^2 \Omega_j \,, \end{aligned} \tag{4}$$

and the new-vacuum state, $|\tilde{0}\rangle$, defined as

$$|\tilde{0}\rangle = \prod_{j\,\nu>0} \left(U_j + V_j\, c^{+}_{j\nu}\, (-1)^{j-\nu}\, c^{+}_{j\,-\nu}\right) |0\rangle \; .$$

Writing n_j and a_j^{+} in terms of quasi-particles

$$n_j = 2V_j^2 \Omega_j + 2U_jV_j\, \Omega_j^{\frac{1}{2}} \left(A_j^{+} + A_j\right) + \left(U_j^2 - V_j^2\right) N_j$$

$$a_j^{+} = U_j^2 A_j^{+} - V_j^2 A_j + \Omega_j^{\frac{1}{2}} U_j V_j \left(1 - N_j/\Omega_j\right) \tag{5}$$

eq. (2) becomes, introducing parameter λ, the Fermi-energy,

$$H - \lambda \bar{n} = H_0 + H_1 + H_c + H_r + H_x$$

where $\bar{n} = \sum_j n_j$,

$$H_0 = \sum_j (e_j - \lambda)\, \Omega_j\, 2V_j^2 - \bar{\Delta}^2/G \; ,$$

$$H_1 = \sum_j E_j N_j \; ,$$

$$H_c = -G \sum_{ij} \Omega_i^{\frac{1}{2}} \Omega_j^{\frac{1}{2}} \chi_i \chi_j \left(U_i^2 A_i^{+} - V_i^2 A_i\right)\left(U_j^2 A_j - V_j^2 A_j^{+}\right) , \tag{6}$$

$$H_r = G \sum_{ij} \chi_i \chi_j U_i V_i\, \Omega_j^{\frac{1}{2}} \left\{ N_i \left(U_j^2 A_j - V_j^2 A_j^{+}\right) + \left(U_j^2 A_j^{+} - V_j^2 A_j\right) N_i \right\} ,$$

$$H_x = -G \sum_{ij} \chi_i \chi_j U_i V_i\, U_j V_j\, N_i N_j \; .$$

The following notation has been introduced:

$$\bar{\Delta} = \Delta_j / \chi_j \quad , \text{ independent of } j$$

$$N_j = \sum_\nu \alpha^+_{j\nu} \alpha_{j\nu}$$

$$A^+_j = 2^{-\frac{1}{2}} \sum_\nu \langle j\nu j -\nu | jj00 \rangle \, \alpha^+_{j\nu} \, \alpha^+_{j-\nu} \, .$$

It is useful to have, also, the identities inverse to eqs. (5).

$$\begin{aligned} N_j &= -2 U_j V_j \Omega_j^{\frac{1}{2}} (a^+_j + a_j) + (U_j^2 - V_j^2) n_j + 2 V_j^2 \Omega_j \\ A^+_j &= U_j^2 a^+_j - V_j^2 a_j - \Omega_j^{\frac{1}{2}} U_j V_j (1 - n_j/\Omega_j) \end{aligned} \tag{5a}$$

The quasi-boson approximation rests on the observation that, if the coefficients of quasi-particle terms in all state vectors are small, then the A^+_j have boson commutation relations, approximately.

$$[A_i \, , A^+_j] = \delta_{ij} (1 - N_j/\Omega_j) \approx \delta_{ij} \tag{7}$$

The approximate equality sign, $\approx$, will be used henceforward to denote equality except for terms of order $\langle N_j \rangle / \Omega_j$ compared to 1.

The quasi-boson approximation consists in approximately linearizing H by finding operators

$$Q^{(k)+} = \sum_j (\psi_j^{(k)} A^+_j - \varphi_j^{(k)} A_j) \qquad k = 0, 1, 2, \ldots \tag{8}$$

which have the property

$$[H, Q^{(k)+}] \approx W^{(k)} Q^{(k)+} + Z^{(k)} \tag{9}$$

where $Z^{(k)}$ denotes terms outside of the space spanned by the A_j^+ and A_j. The original application of the quasi-boson method to pairing[1]) assumed that

$$H - \lambda \bar{n} \approx H_0 + H_1 + H_c$$

since H_r and H_x contain operators N_j, and also are in ratio $1/\sqrt{\Omega_j}$ compared to H_c. However, for deformed nuclei, and for some levels in spherical nuclei, Ω_j is equal to or near unity. Moreover, the terms H_c, H_r, and H_x are not normal-ordered; they have non-zero ground-state expectation values. Also the commutators of H_r and H_x with $Q^{(k)+}$ are not outside of the space spanned by the A_j^+ and A_j. The real utility of writing the Hamiltonian in the form of eq. (6) and then ignoring H_r and H_x seems to be that one thus is guaranteed a complete set of real boson solutions $Q^{(k)+}$. With this form, a zero-energy root is always present. The validity of this formalism must, however, ultimately be established by the direct numerical comparison of its results with exact results in simple soluble systems. Such a comparison is made in section 7.

Performing the commutation, (9), ignoring $Z^{(k)}$, H_r, and H_x gives

$$(2E_j - W^{(k)})\psi_j^{(k)} - G\chi_j(U_j^2 - V_j^2)\Omega_j^{\frac{1}{2}}\rho^{(k)} - G\chi_j\Omega_j^{\frac{1}{2}}\theta^{(k)} = 0$$

$$(2E_j + W^{(k)})\varphi_j^{(k)} - G\chi_j(U_j^2 - V_j^2)\Omega_j^{\frac{1}{2}}\rho^{(k)} + G\chi_j\Omega_j^{\frac{1}{2}}\Theta^{(k)} = 0 \quad (10)$$

where

$$\rho^{(k)} = \frac{1}{2}\sum_j \chi_j \Omega_j^{\frac{1}{2}}(U_j^2 - V_j^2)(\psi_j^{(k)} + \varphi_j^{(k)}),$$

$$\Theta^{(k)} = \frac{1}{2}\sum_j \chi_j \Omega_j^{\frac{1}{2}}(\psi_j^{(k)} - \varphi_j^{(k)}). \quad (11)$$

Solving eqs. (10) for $\psi_j^{(k)}$ and $\varphi_j^{(k)}$ and substituting in eqs. (11) gives

$$\rho^{(k)} = G\sum_j \chi_j^2 \Omega_j \frac{2(e_j - \lambda)^2 \rho^{(k)} + W^{(k)}(e_j - \lambda)\Theta^{(k)}}{E_j(4E_j^2 - W^{(k)2})},$$

$$\Theta^{(k)} = G\sum_j \chi_j^2 \Omega_j \frac{W^{(k)}(e_j - \lambda)\rho^{(k)} + 2E_j^2\Theta^{(k)}}{E_j(4E_j^2 - W^{(k)2})}.$$

For $\bar{\Delta} \neq 0$, these linear, simultaneous equations in $\rho^{(k)}$ and $\theta^{(k)}$ have a non-trivial solution only if

$$(1 - h^{(k)})W^{(k)2}d^{(k)} + W^{(k)2}g^{(k)2} = 0 \quad (12)$$

where $$d^{(k)} = G \sum_j \chi_j^2 \Omega_j \left[2E_j \left(4E_j^2 - W^{(k)2} \right) \right]^{-1} ,$$

$$g^{(k)} = G \sum_j \chi_j^2 \Omega_j (e_j - \lambda) \left[E_j \left(4E_j^2 - W^{(k)2} \right) \right]^{-1} ,$$

$$h^{(k)} = G \sum_j \chi_j^2 \Omega_j 2 (e_j - \lambda)^2 \left[E_j \left(4E_j^2 - W^{(k)2} \right) \right]^{-1} .$$

Reserving the zero root for later consideration, if $W^{(k)} \neq 0$, eq. (12) becomes

$$\left(1 - h^{(k)} \right) d^{(k)} + g^{(k)2} = 0 . \tag{13}$$

The ratio, $\theta^{(k)}/\rho^{(k)}$ at a root is

$$\frac{\theta^{(k)}}{\rho^{(k)}} = - \frac{g^{(k)}}{W^{(k)} d^{(k)}} = \frac{\left(1 - h^{(k)} \right)}{W^{(k)} g^{(k)}} . \tag{13a}$$

If $\chi_j = 1$, all j, (constant pairing force) secular equation (13) simplifies to

$$\sum_j \Omega_j \left[E_j \left(y^{(k)} - 2 (e_j - \lambda) \right) \right]^{-1} = 0 \tag{14}$$

where the roots, $y^{(k)}$, are related to the positive-energy solutions, $W^{(k)}$, by

$$W^{(k)} = + \left(y^{(k)2} + 4 \bar{\Delta}^2 \right)^{\frac{1}{2}} . \tag{15}$$

For constant pairing

$$\frac{\Theta^{(k)}}{\rho^{(k)}} = \frac{y^{(k)}}{W^{(k)}} \tag{16}$$

(Eqs. (14), (15), (16) are true <u>only</u> in the case of a <u>constant</u> pairing potential).

The case of a trivial solution to eqs. (4), $\bar{\Delta} = 0$, $G \neq 0$, is best treated separately. The secular equation is

$$\frac{1}{G} = \sum_{e_j<\lambda} \frac{\chi_j^2 \Omega_j}{(\omega^{(k)} + 2E_j)} - \sum_{e_j>\lambda} \frac{\chi_j^2 \Omega_j}{(\omega^{(k)} - 2E_j)} \tag{17}$$

where the roots, $\omega^{(k)}$, are related to the positive $W^{(k)}$ roots by

$$W^{(k)} = |\omega^{(k)}|$$

and where $$\frac{\Theta^{(k)}}{\rho^{(k)}} = \mathrm{sgn}(\omega^{(k)}) \quad .$$

In the trivial ($\bar{\Delta} = 0$) case, $Q^{(k)+}$ becomes a sum of two real particles and two real holes. There is, in general, no zero-energy root. For $\bar{\Delta} = 0$, the first excited state is a two-boson state.

The eigen-operators $Q^{(k)+}$ (eq. (8)) are determined by

$$\psi_j^{(k)} = \frac{\chi_j \Omega_j^{\frac{1}{2}}}{2E_j - W^{(k)}} \left[\frac{e_j - \lambda}{E_j} + \frac{\Theta^{(k)}}{\rho^{(k)}} \right] \rho^{(k)} ,$$

$$\varphi_j^{(k)} = \frac{\chi_j \Omega_j^{\frac{1}{2}}}{2E_j + W^{(k)}} \left[\frac{e_j - \lambda}{E_j} - \frac{\Theta^{(k)}}{\rho^{(k)}} \right] \rho^{(k)} . \tag{18}$$

Since H is hermitian, $W^{(k)} \neq W^{(k')}$ implies

$$[Q^{(k)}, Q^{(k')+}] \approx [Q^{(k)}, Q^{(k')}] \approx 0 \quad . \tag{19}$$

The factor $\rho^{(k)}$ is chosen so that

$$\sum_j \left(\psi_j^{(k)} \psi_j^{(k')} - \varphi_j^{(k)} \varphi_j^{(k')} \right) = \delta_{kk'} \quad . \tag{20}$$

Also, from eq. (19),

$$\sum_j \left(\psi_j^{(k)} \varphi_j^{(k')} - \varphi_j^{(k)} \psi_j^{(k')} \right) = 0 \quad . \tag{21}$$

3. The Ground State

The ground-state vector, denoted $|gnd\rangle$, is defined by

$$Q^{(k)} |gnd\rangle \approx 0 \quad ; \quad R^{(0)} |gnd\rangle \approx 0 \tag{22}$$

where k = 1,2,... and $R^{(0)+}$ is the zero-energy boson to be described later (section 4). Consider $\psi_j^{(k)}$ to be the kj$\underline{\text{th}}$ entry of the square matrix ψ, and similarly for $\varphi_j^{(k)}$:

$$[\psi]_{kj} = \psi_j^{(k)} \quad , \quad [\varphi]_{kj} = \varphi_j^{(k)} \quad .$$

The zero-energy root, $R^{(0)+}$, is denoted by k = 0, i.e., $W^{(0)} = 0$. The index k runs from 0 to L-1, where L is the number of j-levels. Then eq. (21) implies that

$$\beta = [\psi]^{-1}[\varphi] \tag{23}$$

is a symmetric matrix: $\beta_{ij} = \beta_{ji}$.

Thus

$$|gnd\rangle = K\, e^{\frac{1}{2}\sum_{ij}\beta_{ij}A_i^+A_j^+}\,|\tilde{0}\rangle \tag{24}$$

has property (22). The normalization factor, K, is given by

$$K = e^{-\frac{1}{4}(\mathrm{Tr}\,\beta^2)} .$$

From the form of eq. (24) it is clear that the basic condition for validity of the quasi-boson approach, $\langle N_j\rangle/\Omega \ll 1$, will be satisfied only if $\beta_{ij} \ll 1$. If β_{ij} is not small, a large four-quasi-particle term $\beta_{ij}A_i^+A_j^+$ will appear in the ground state.

Although, as mentioned, the zero-energy solution, k = 0, is in general required to make $[\psi]$ and $[\varphi]$ square, it is, in certain cases, possible to do without it. Consider the set of quantities

$$M_{0j}([\varphi])$$

the signed minors of the first row of matrix $[\varphi]$. Remove the first rows (k = 0) from both $[\psi]$ and $[\varphi]$ and replace them by M_{0j} and zeros respectively. Then if the $\varphi_j^{(k)}$ are <u>uniformly</u> less than the $\psi_j^{(k)}$ the matrix

$$\beta' = [\psi']^{-1}[\varphi']$$

will be symmetric and small. (The modified matrices are denoted by primes.) The method will not be reliable for small G values when <u>some</u> $\psi_j^{(k)}$ may be small compared to some $\varphi_j^{(k)}$. The matrix β may then be symmetric and large.

4. Zero-energy Bosons

To find the eigen-operator of the root $W^{(0)}$, notice that eqs. (13a) imply that $\rho^{(0)}/\theta^{(0)} = 0$ when $W^{(0)} = 0$. Thus, from (18)

$$Q^{(0)+} = \frac{G}{2} \sum_j \frac{\chi_j \Omega_j^{\frac{1}{2}}}{E_j} \left(A_j^+ + A_j\right) \Theta^{(0)} . \tag{25}$$

It is instructive also to derive this eigen-operator directly. Try

$$Q^{(0)+} = \sum_j \bar{\Psi}_j^{(0)} \left(A_j^+ + A_j\right)$$

$$\text{with} \quad \bar{\varphi}_j^{(0)} = - \bar{\Psi}_j^{(0)}$$

where $\bar{\Psi}_j^{(0)}$ is an unknown coefficient to be determined. Then

$$\left[(H_1+H_c), Q^{(0)+}\right] \approx \sum_j \left(2E_j \bar{\Psi}_j^{(0)} - G\chi_j \Omega_j^{\frac{1}{2}} \Theta^{(0)}\right)\left(A_j^+ - A_j\right) \tag{26}$$

will be zero if

$$\bar{\Psi}_j^{(0)} = \frac{G}{2} \frac{\chi_j \Omega_j^{\frac{1}{2}}}{E_j} \Theta^{(0)}$$

which is equivalent to (25). The consistency condition for $\theta^{(0)}$ to be non-zero, eq. (11), is then the same as the eq. (4) used to define λ and $\bar{\Delta}$.

The form of the operator on the right-hand-side in eq. (26) and the fact that $Q^{(0)+}$ is hermitian, suggest that another boson, needed for completeness, can be found to be of the form

$$P^{(0)+} = \sum_j \bar{\bar{\Psi}}_j^{(0)} (A_j^+ - A_j)$$

$$\text{with} \quad \bar{\bar{\varphi}}_j^{(0)} = \bar{\bar{\Psi}}_j^{(0)} \quad . \tag{27}$$

By a process similar to that just used to derive $Q^{(0)+}$, a skew-hermitian boson, $P^{(0)+}$, can be found which satisfies

$$\left[(H_1 + H_c), P^{(0)+} \right] \approx 2 \bar{\Delta} Q^{(0)+} \tag{28}$$

and consistency condition $\rho^{(0)} \neq 0$. (Eq. (11))
It is defined by (27) with

$$\bar{\bar{\Psi}}_j^{(0)} = \frac{G}{2} \frac{\chi_j \Omega_j^{\frac{1}{2}}}{E_j^2} \left(\bar{\Delta} + (e_j - \lambda) \frac{s}{r} \right) \Theta^{(0)} \tag{29}$$

where

$$r = \sum_j \chi_j^4 \Omega_j \frac{\bar{\Delta}}{E_j^3} ,$$

$$s = \sum_j \chi_j^2 \Omega_j \frac{e_j - \lambda}{E_j^3} .$$

Eqs. (9), (19), and (28) are sufficient to imply

$$\begin{aligned} [Q^{(k)}, Q^{(0)+}] &\approx 0 \qquad k \neq 0 \\ [Q^{(k)}, P^{(0)+}] &\approx 0 \qquad k \neq 0 . \end{aligned} \tag{30}$$

Hence, although $Q^{(0)+}$ is the actual solution to the quasi-boson equations, a symmetric β-matrix (eq. (23)) and an orthonormal non-zero-energy boson spectrum (orthogonal to the ground-state, to the spurious boson $Q^{(0)+}$, and to $P^{(0)+}$) will result if one uses as the zero-energy boson any linear sum of $Q^{(0)+}$ and $P^{(0)+}$; if instead of $Q^{(0)+}$, one uses

$$R^{(0)+} = Q^{(0)+} + f P^{(0)+} ,$$

$$\text{ie.,} \quad R^{(0)+} = \sum_j \left(\psi_j^{(0)} A_j^+ - \varphi_j^{(0)} A_j \right)$$

with (31)

$$\psi_j^{(0)} = \bar{\psi}_j^{(0)} + f \bar{\bar{\psi}}_j^{(0)} ,$$

$$\varphi_j^{(0)} = - \bar{\psi}_j^{(0)} + f \bar{\bar{\psi}}_j^{(0)} .$$

The normalizing factor in eqs. (25) and (29), $\theta^{(0)}$, should be chosen so that

$$[R^{(0)}, R^{(0)+}] \approx 1 \quad .$$

Although $R^{(0)+}$ is orthogonal to the non-zero-energy spectrum,

$$[Q^{(k)}, R^{(0)+}] \approx 0 \qquad k \neq 0 \quad , \tag{32}$$

$R^{(0)+}$ is not <u>in general</u> a valid eigen-operator of H:

$$[(H_1 + H_c), R^{(0)+}] \approx 2\bar{\Delta} f \, Q^{(0)+} \quad . \tag{33}$$

As noted above, the success of the theory in general does not require that the $R^{(0)+}$ used in eq. (22) be an eigen-operator.

However, for small values of $\bar{\Delta}$, $R^{(0)+}$ is <u>approximately</u> an eigen-operator of H. The coefficients of $Q^{(0)+}$, eq. (25), are chosen to be at most of order unity for G small, ($G' \ll 1$).† Since f will be chosen to be similarly bounded, (eq. 36), the right hand

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† The G' is a dimensionless force parameter defined by

$$G' \equiv G/G_c$$

where G_c is the critical G-value at the nearest closed j-shell. For non-closed-shell nuclei, G_c is defined as approximately the minimum point of the boson-energy versus G curve. See the discussion in section 7-7.10.

side of (33) will be approximately zero compared to the rest of the boson energies whenever $\bar{\Delta}/W^{(k)} \ll 1$, $(k \neq 0)$, as is in general true for small G. This approximate property will allow $R^{(0)+}$ to become part of the boson excitation spectrum in the case $G' \ll 1$.

The <u>necessity</u> for some boson of the form (31) to play a role in the excitation spectrum can be seen by considering the limit $G' \ll 1$ in a case in which the average particle number, n, does not exactly fill the j-shell nearest the fermi-surface. In this case $G \neq 0$ implies $\bar{\Delta} \neq 0$, and as G' becomes small the fermi-energy, λ, approaches infinitesimally close to one of the e_j's. Denote this e_j by the subscript λ,

$$\lim_{G' \ll 1} \lambda = e_\lambda .$$

The secular equation for constant pairing, eq. (14), can be graphed, and in this limit is shown in fig. 1. For concreteness a case of four j-levels has been shown, with the second level as e_λ. The roots $y^{(k)}$ have been labeled by the value of $2(e_j - \lambda)$ which they approach in the $G' \ll 1$ limit. (The previous notation has been changed somewhat to denote the j-levels 1,2,3,4 instead of 3/2, 7/2 etc.) In the limit $G' \ll 1$, the boson operator $Q^{(k)+}$ reduces to the quasi-particle creation operator corresponding to the $k^{\underline{th}}$ root

$$\lim_{G' \ll 1} \left(Q^{(k)+} - A_{j=k} \right) = 0$$

where $j = k$ as explained above.

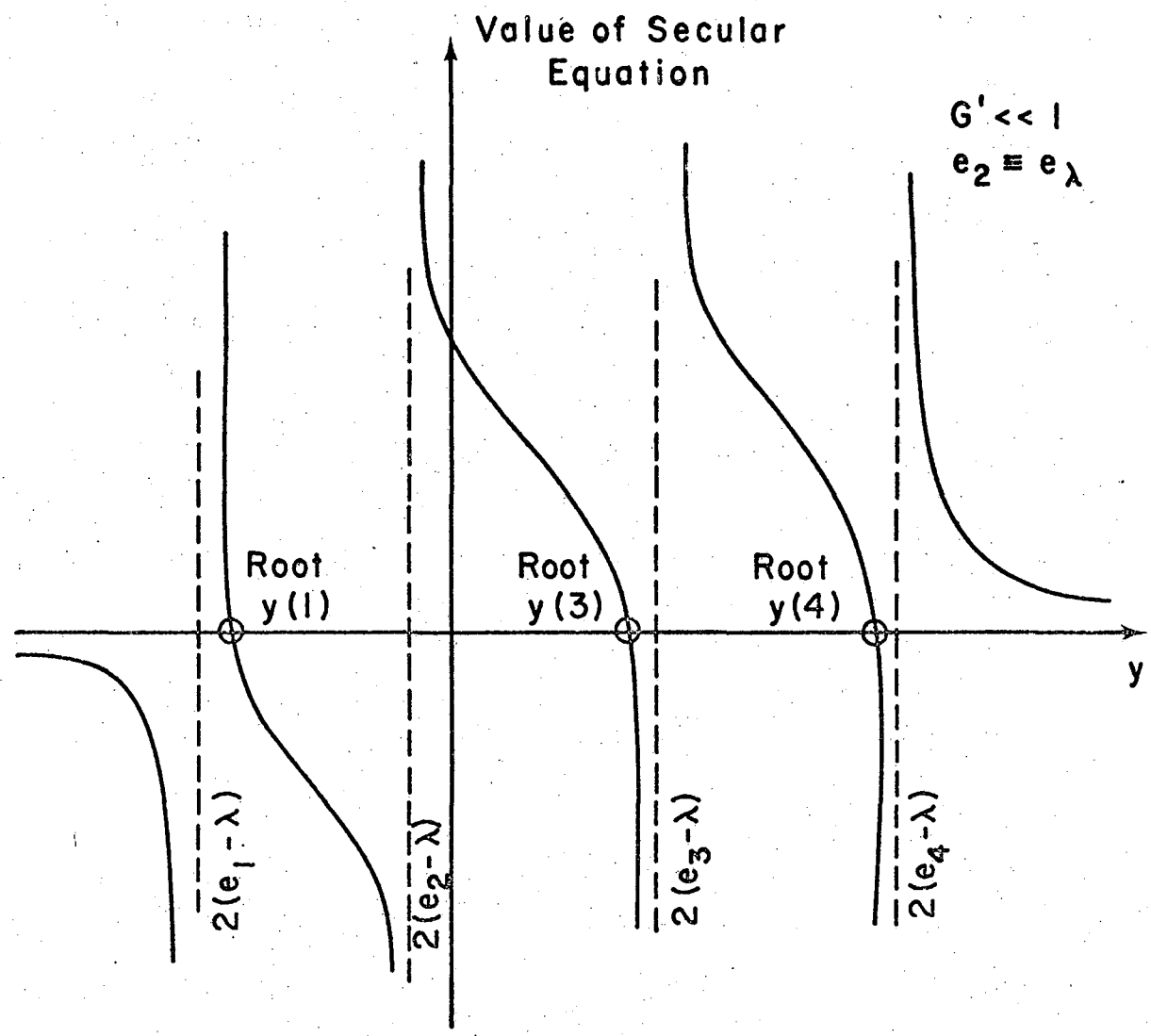

Fig. 1

Schematic graph of the secular equation, eq. 14, for a four level system in the $G' \ll 1$ limit.

This corresponds to the fact that as $G' \ll 1$, the excitation spectrum must reduce simply to particle and hole operators. However, A_2^+ is missing, and its place must be filled by some combination of the only other available bosons, $Q^{(0)+}$ and $P^{(0)+}$. Hence the zero-energy boson must in certain cases be a legitimate member of the boson spectrum.

Although fig. 1 shows a particular case, the result is general. The boson A_λ^+ will always be missing from the non-zero-energy-boson spectrum in the $G' \ll 1$ limit; and eq. (33) shows that, in that limit, any boson of the form (31) is an approximate eigen-operator of H. This paper will conclude that, if function "f" is defined properly, the zero-energy boson, $R^{(0)+}$, will also be the missing member of the excitation spectrum. Thus the boson ground state will be defined by eq. (22) and, in the $G' \ll 1$ limit, the same $R^{(0)+}$ as used there will obey

$$\lim_{G' \ll 1} \left(R^{(0)+} - A_\lambda^+ \right) = 0$$

where A_λ^+ is the missing boson.†

However, the usual practice[3,4]) in beta-vibration calculations has been to use $Q^{(0)+}$ as the zero-energy boson. This corresponds

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† The numerical section 7 (in particular figs. 11 and 12) indicates that the boson $R^{(0)+}$ may be useful for G' near 1 and not only for $G' \ll 1$ as in the argument given here.

to f = 0 in the present notation. Since $Q^{(0)+}$ is hermitian, the missing boson in the G'<<1 excitation spectrum must then be $P^{(0)+}$. It is easy to see from eqs. (22), (25), and (27) that when G'<<1,

$$\lim_{G'\ll 1}\left(P^{(0)+}|gnd\rangle - 2\,\bar{\bar{\Psi}}^{(0)}_{\lambda} A^{+}_{\lambda}|gnd\rangle\right) \approx 0$$

which is indeed the missing boson. The difficulty with this practice is that $Q^{(0)+}$, being hermitian, has a non-vanishing destruction-operator term for all values of G'. This destruction part of $Q^{(0)+}$ introduces correlations into the ground-state even in the limits G'>>1 and G'<<1. Thus, for example when all $\chi_j = 1$,

$$\lim_{G'\ll 1}\left(|gnd\rangle - K e^{-\frac{1}{2}(A^{+}_{\lambda})^{2}}|\tilde{o}\rangle\right) = 0$$

$$\lim_{G'\gg 1}\left(|gnd\rangle - K e^{-\frac{1}{2}\sum_{ij}\frac{\Omega_i^{\frac{1}{2}}\,\Omega_j^{\frac{1}{2}}}{\Omega}A^{+}_{i}A^{+}_{j}}|\tilde{o}\rangle\right) = 0 \quad ,$$

where $\Omega = \sum_j \Omega_j$.

In the limit, G'<<1, the effect is to introduce large four, eight, etc. quasi-particle terms into the ground state in violation of the central assumption of the theory, eq. (7). In the limit, G'>>1, the effect is more subtle. While $\sqrt{\Omega_i}\,\sqrt{\Omega_j}/\Omega$ may be of order unity for some levels of spherical nuclei, it will usually be small for deformed nuclei. Instead of large terms, β_{ij}, the effect

here is a kind of complementarity between energy and particle number. As shown in the next section (eq. (40)), use of $Q^{(0)+}$ as the zero-boson is equivalent to requiring particle number to be a good quantum number, in the quasi-boson sense. That is

$$(\bar{n} - n)|gnd\rangle \approx 0 \quad . \tag{35}$$

A one boson state is in general a sum of the ground, first-excited, second-excited, etc., states of systems of n, n ± 2, n ± 4, etc. particles. The effect of eq. (35) is to restrict the spread of the ground and boson states in n. Because of the limited number of degrees of freedom of the quasi-particle and quasi-boson approximations, this constriction in n is accompanied by a greater spreading in energy, resulting in a larger ground and second-excited state component in the lowest one-boson state, etc. This effect can be seen numerically in the simple model-spherical system studied in section 7. Comparison of fig. 6a with fig. 6b shows the effect. It can be argued that this effect will be much less in deformed nuclei. However it is also true that in deformed nuclei the energy levels are more closely spaced and hence a smaller uncertainty in energy will still mix several neighboring exact 0+ states into each boson.

If, instead of f = 0, a function f is used having the following limits†

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† Eqs. (36b) and (37b) are approximate relations which are exact for the case of constant pairing force (all $\chi_j = 1$). Thus for these equations only, the approximate equality sign is used in a sense different from that of eq. (7).

$$\lim_{G'<<1}\left(f - \frac{2\bar{\Delta}}{G\,\Omega_\lambda}\right) = 0 \tag{36a}$$

$$\lim_{G'>>1} f \approx 1 \tag{36b}$$

then the ground state defined by eq. (22) will obey

$$\lim_{G'<<1}\left(|\mathrm{gnd}\rangle - |\tilde{0}\rangle\right) = 0 \tag{37a}$$

$$\lim_{G'>>1}\left(|\mathrm{gnd}\rangle - |\tilde{0}\rangle\right) \approx 0 \tag{37b}$$

and also the boson defined by eq. (31) will obey

$$\lim_{G'<<1}\left(R^{(0)+} - A_\lambda^+\right) = 0\,, \quad \text{where } A_\lambda^+ \text{ is} \tag{38}$$

the missing boson.

The form of function, f, between these limits is suggested by arguments in the next section. It is

$$f = \frac{a}{b} \tag{39}$$

where

$$a = \sum_j \bar{\Psi}_j^{(0)}\,\bar{\bar{\Psi}}_j^{(0)}$$

and

$$b = \sum_j \left(\bar{\bar{\Psi}}_j^{(0)}\right)^2 .$$

This function fulfills conditions (36). The zero-frequency boson is then, not $Q^{(0)+}$, but that given in eq. (31), and this same boson, $R^{(0)+}$, is part of the boson excitation spectrum for $G'<<1$.

5. The Spurious States

The meaning of zero-energy boson, $Q^{(0)+}$, is obtained by writing the first of eqs. (5) in the following form, using (4) and (25):

$$\bar{n} - n = \frac{2\bar{\Delta}}{G} Q^{(0)+} + \sum_j (U_j^2 - V_j^2) N_j$$

$$\text{or} \qquad \bar{n} - n \approx \frac{2\bar{\Delta}}{G} Q^{(0)+} . \tag{40}$$

Boson $Q^{(0)+}$ is that operator which would be approximately zero if particle number were a good quantum number.

The meaning of boson $P^{(0)+}$ is only slightly more obscure. Eqs. (4) imply the following differential forms

$$dG = \frac{G^2}{2}\left(-s\, d\lambda + r\, d\bar{\Delta}\right)$$

$$dn = \bar{\Delta}\left(t\, d\lambda + s\, d\bar{\Delta}\right) \tag{41}$$

where r, s are the function defined earlier, in eqs. (29), and t is defined

$$t = \sum_j \frac{\gamma_j^2\, \Omega_j\, \bar{\Delta}}{E_j^3} . \tag{42}$$

Eqs. (41) can be inverted, allowing the calculation of the changes in various quantities as n is changed slightly, with G fixed.

Thus
$$\left.\frac{dA_j^+}{dn}\right)_G dn \approx -d\gamma\, \bar{\bar{\psi}}_j^{(0)} ,$$

where
$$d\gamma = \frac{1}{G\,\Theta^{(0)}} \left.\frac{d\lambda}{dn}\right)_G dn \tag{43}$$

and where eqs. (5), (5a) have been used, and operators a_j^+ and n_j have been considered constant in the differentiation. Coefficient $\bar{\bar{\psi}}_j^{0}$ is the same as that defining $P^{(0)+}$ in eq. (29). Thus, if n is changed to n' = n + dn,

$$A_j^+ \longrightarrow A_j^{+\prime} = A_j^+ + \left.\frac{dA_j^+}{dn}\right)_G dn$$

and the original vacuum state, $|\tilde{0}\rangle$, defined by

$$A_j\,|\tilde{0}\rangle = 0 \quad , \quad \text{all } j \quad ,$$

becomes, to first order in dn,

$$|\tilde{0}\rangle' = \left(1 + d\gamma \sum_j \bar{\bar{\psi}}_j^{(0)} A_j^+\right) |\tilde{0}\rangle \tag{44}$$

where $|\tilde{0}\rangle'$ is defined by

$$A_j^{+\prime}\,|\tilde{0}\rangle' = 0 \quad , \quad \text{all } j \; .$$

The creation operator part of operator $P^{(0)+}$ is thus the <u>primitive number fluctuation</u> which connects $|\tilde{0}\rangle$ at n to $|\tilde{0}\rangle'$ at

$n' = n + dn$.† The word <u>primitive</u> is used to indicate that, so far, no use has been made of the parts of the Hamiltonian beyond H_1. (i.e., H_c has not been used.)

It is interesting to conjecture also a <u>primitive pairing vibration</u> derived similarly from

$$\left.\frac{dA_j^+}{dG}\right)_n dG \approx d\eta\ \psi_j^{(P)}$$

where
$$\psi_j^{(P)} = \frac{G\chi_j\,\Omega_j^{\frac{1}{2}}}{2E_j^2}\left(\bar{\Delta}\,\frac{s}{t} - (e_j - \lambda)\right) \tag{45}$$

and
$$d\eta = \frac{1}{G}\left.\frac{d\bar{\Delta}}{dG}\right)_n dG \quad .$$

Denoting by $|\tilde{o}\rangle''$ the vacuum state at $G'' = G + dG$,

$$|\tilde{o}\rangle'' = \left(1 - d\eta \sum_j \psi_j^{(P)} A_j^+\right)|\tilde{o}\rangle \tag{46}$$

as above. The two differential operators in (44) and (46) are not orthogonal. However the operator in (46) is orthogonal to $Q^{(0)+}$. This primitive pairing vibration is calculated in the numerical section of the paper (see fig. 15). It might be expected that the primitive-pair-vibration would be spread over the one-boson states as a kind of strength function. However it appears numerically

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† A similar result was obtained by Bès[4]).

that it is almost identical to the two-boson state in the simple example calculated. (See fig. 14) The general result would therefore be that the primitive pair vibration spreads over the <u>two</u>-boson states. This result, although interesting, seems not to be very useful, since the two-boson state itself is spread over several levels of the actual excitation spectrum.

Now introduce H_c and the quasi-boson formalism and examine the change in the boson ground state when $n \rightarrow n' = n + dn$. Each boson $Q^{(k)+}$ changes to $Q^{(k)+'}$ where

$$Q^{(k)+'} = Q^{(k)+} + dX^{(k)} - \delta_{k0}\, dc^{(k)}$$

where
$$dX^{(k)} = \sum_j \left(A_j^+ d\psi_j^{(k)} - A_j\, d\varphi_j^{(k)} \right) \tag{47}$$

and
$$dc^{(k)} = \sum_j \left(\psi_j^{(k)} - \varphi_j^{(k)} \right) \bar{\bar{\psi}}_j^{(0)}\, d\gamma \quad .$$

Recalling that (eq. (24))

$$|gnd\rangle = B^+ |\tilde{o}\rangle \quad ,$$

where
$$B^+ = K\, e^{\frac{1}{2}\sum_{ij} \beta_{ij} A_i^+ A_j^+} \quad , \tag{24a}$$

and eq. (44), write

$$|gnd\rangle' = \left(1 + dY\right) B^+ |\tilde{o}\rangle' \tag{48}$$

where

$$dY = \sum_{k \neq 0} dp_k\, Q^{(k)+} + dp_0\, R^{(0)+} \quad .$$

Determine the dp_k by the conditions

$$Q^{(k)\prime} \, |gnd\rangle' \approx 0 \quad , \quad R^{(0)\prime} \, |gnd\rangle' \approx 0 \quad .$$

The result is

$$dp_k = -d\gamma \sum_j \bar{\bar{\Psi}}_j^{(0)} \varphi_j^{(k)} \quad , \quad k \neq 0 \quad , \tag{49a}$$

$$dp_0 = d\gamma (f\, b - a) \tag{49b}$$

where a and b are defined in eqs. (39).

The factor multiplying $d\gamma$ in (49a) is small, compared to unity, in the large and small G' limits. The equation (49b) can be made to vanish identically if

$$f = \frac{a}{b} \quad . \tag{39a}$$

Thus the effect of the change in $Q^{(k)+}$ and $R^{(0)+}$ on the ground state can be minimized. That is, if eq. (39a) holds,

$$|gnd\rangle' = \left(1 + \sum_{k \neq 0} dp_k \, Q^{(k)+}\right) B^+ \, |\tilde{0}\rangle'$$

which is nearly equal to, simply,

$$|gnd\rangle' = B^+ \, |\tilde{0}\rangle' \quad .$$

In this derivation, matrix β has been assumed small enough that <u>changes</u> in B^+ can be ignored. Also operators $dX^{(k)+}$ have been ignored.

The function f in eq. (39a) is the same as that defined by eq. (39) and discussed in section 4. Eq. (39) (or (39a)) is used to determine the function, f, which is then used to define the zero-energy boson

$$R^{(0)+} = Q^{(0)+} + f\, P^{(0)+} \quad .$$

The results of this definition are compared with the usual form of the theory (f = 0) in the numerical part, section 7.

6. A Necessary Refinement

It has been shown in the previous two sections that boson $R^{(0)+}$, the zero-energy root, becomes part of the excitation spectrum when $\bar{\Delta} \neq 0$ and $G' \ll 1$. This corresponds to the fact that, for $G' = 0$, the ground state is simply the shell-model state, and the lowest excited 0+ states are simply un-mixed, two-particle, two-hole configurations. The first excited state, for example, at $G' = 0$ may be of the form

$$a_j^+ \, a_\lambda \, |\text{ground state}\rangle$$

where a_j^+ is defined in eq. (3).
The quasi-particle operators A_j^+ become particles or holes when they are well above or below the fermi-level respectively:

$$e_j \gg \lambda \qquad A_j^+ \longrightarrow a_j^+$$

$$e_j \ll \lambda \qquad A_j^+ \longrightarrow -a_j \quad .$$

This follows, of course, from eq. (5a) and the vanishing of $U_j V_j$ for these levels.

However, it is an essential difficulty of the quasi-particle method that, for the level at the fermi surface in the $G' \ll 1$ limit (the partially-filled level, denoted e_λ in section 4)

$$\lim_{G' \ll 1} U_\lambda V_\lambda \neq 0 \quad .$$

It then is impossible to represent either a_λ^+ or a_λ in terms of quasi-particle operators A_λ^+ and A_λ. Instead, eq. (5) shows

$$\begin{aligned} a_\lambda^+ &\approx U_\lambda^2 A_\lambda^+ - V_\lambda^2 A_\lambda + \Omega_\lambda^{\frac{1}{2}} U_\lambda V_\lambda \\ a_\lambda &\approx -V_\lambda^2 A_\lambda^+ + U_\lambda^2 A_\lambda + \Omega_\lambda^{\frac{1}{2}} U_\lambda V_\lambda \, . \end{aligned} \tag{50}$$

As noted, this is an essential difficulty of the whole quasi-particle approach. The quasi-boson extension of the quasi-particle theory does not solve it.

However, it follows from eqs. (37) and (38) that, when one uses (31) and (39) to define $R^{(0)+}$, the operators

$$\begin{aligned} S^{(0)+} &= R^{(0)+} - \Omega_\lambda^{\frac{1}{2}} \frac{U_\lambda}{V_\lambda} \\ T^{(0)+} &= R^{(0)+} + \Omega_\lambda^{\frac{1}{2}} \frac{V_\lambda}{U_\lambda} \end{aligned} \tag{51}$$

have limits

$$\lim_{G' \ll 1} V_\lambda^2 \, S^{(0)+} \approx -a_\lambda$$

$$\lim_{G' \ll 1} U_\lambda^2 \, T^{(0)+} \approx a_\lambda^+ \quad .$$

Since constants commute with every operator, the addition of a constant to $R^{(0)+}$ does not invalidate it as a zero-energy boson (i.e., the discussion of eq. (33) still holds true).

Thus after normalization, the proper first excited state operator in the $G' \ll 1$ limit consists of $S^{(0)+}$ or $T^{(0)+}$ multiplied by some non-zero-energy boson. The choice of $S^{(0)+}$ or $T^{(0)+}$ depends on the single-particle energy level spacings.

Although this procedure has to be considered a piece of patchwork, it is nonetheless completely general - it can be applied to any system of levels. The numerical examples in section 7 (fig. 11c and fig. 12c) show that the procedure gives good results.

7. Numerical Examples

7.1 THE MODEL SYSTEM - The methods outlined in previous sections are here applied to a simple model system† consisting of two j-levels, each with $j = 9/2$. (Since the levels have equal j, they will be labeled by 1 and 2, rather than by j-value.) This system will be considered in the constant-pairing-potential quasi-boson approximation with $n = 8$ and $n = 10$ particles. (To avoid confusion, the letter "n" will be reserved for the vacuum-state expectation value of the number operator, as in eq. (4).) For $n = 10$, the critical G value (below which $\bar{\Delta} = 0$) is $G_c = 0.1$. This corresponds to $G' = 1$, where G' is a dimensionless force parameter defined, as discussed in section 7.10, by

$$G' = \frac{(\Omega_1 + \Omega_2)\, G}{e_2 - e_1} \quad . \tag{52}$$

For $n = 8$, there is no non-zero critical G value.

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† This model system is used to study the accuracy of the quasi-particle vacuum (ground) state in reference[5]). Boson and exact energies are computed for a series of similar model systems in reference[1]).

For this model system, there is only one non-zero-energy boson. It will be denoted

$$Q^{(1)+} \quad , \quad W^{(1)} \neq 0 \quad .$$

There is also a zero-energy boson $R^{(0)+}$, a linear sum of $Q^{(0)+}$ and $P^{(0)+}$, as derived in sections 4, 5. The boson ground and excited states are computed for two different choices of $R^{(0)+}$:

First, $$R^{(0)+} = Q^{(0)+} \qquad (f = 0)$$

and second, $$R^{(0)+} = Q^{(0)+} + f\,P^{(0)+}$$

with function, f, given by eqs. (39). The first choice is that derived by H.-Feldman[1]) and used in published calculations of β-vibrations in deformed nuclei[3,4]). The second is that derived in the present paper. The choice, of course, affects the matrix β (here a 2 x 2 matrix) which defines the boson ground state, eq. (22).

7.2 DISPLAY OF RESULTS OF CALCULATIONS - The constant pairing force is also diagonalized exactly (for the four lowest-energy eigen-vectors) in the above model system - for the cases of every possible even number of particles, m = 0, 2, 4, ..., 20. These diagonalizations are, of course, number conserving. However, the boson states calculated as described above are not eigen-vectors of $\bar{n}$, the number operator. They consist of sums of pieces with every even number of particles from m = 0 to m = 20. For a given

boson state above, the inner products of the m-particle piece with the four exact eigen-vectors of the m-particle system are calculated, for each even m between 0 and 20. These inner products (squared) are displayed on a plot with particle number, m, running along the horizontal axis, and the four excited states running up the vertical axis in ascending order of energy. Each squared-inner-product is followed by the sign of the inner-product before squaring. In this way the original products can be recovered from the figures. For example, in fig. 6a, the inner product of the one-boson state with the exact second-excited 0+ state of the m = 10 system is +0.21 (= $+\sqrt{.044}$). Contour lines are drawn at the 10%, 5% (dotted), and 1% contours. Note that one-percent is still a large coefficient (± 0.1), due to the squaring. Each display is normalized to a summed squared-intensity of unity. This is necessary even after the boson states are normalized in the quasi-boson sense, eq. (20), since eq. (7) is not exact. The sum of squared intensities before normalization is denoted K^2 on each figure. This number, together with the signs, allows one to tell a real state from a spurious one, real states having a coherence of signs of large components and a total pre-normalization intensity of near unity. In all the diagrams, squared products less than 5×10^{-5} are replaced by zeros. Those between 5×10^{-5} and 9.5×10^{-4} are written to four decimal places (one significant); those between 9.5×10^{-4} and 1.0 are written to three decimal places.

7.3 BOSON ENERGIES - Fig. 2 shows the exact excitation energies of the first excited 0+ states for m = 6, 8, and 10 compared with the boson energies for n = 8 and 10. This figure indicates, as do later ones, that the quasi-boson method fails for medium to low force strength ($0.8 < G' < 1.2$) at closed subshells (n = 10 in this case). In this region the boson energy for n = 8 is closer to the m = 10 exact energy than is the n = 10 boson energy. This result suggests the following rule-of-thumb: To calculate approximate energy levels at closed j-shells the average number, n, should be set slightly more or less than the number for shell-closure. This rule does not really introduce n as a new free parameter of the system, since, except for a sharp cusp for small G' at the shell closure, the boson energy is fairly insensitive to n.

7.4 GROUND STATES - The ground states calculated by the various methods above all show a similar pattern. Therefore, the various ground states will be presented here only in one, typical, case: n = 10, G' = 1.6. Fig. 3 shows the quasi-particle vacuum state, i.e., no ground state correlation due to bosons. It is spread over the exact ground states of several adjacent systems, mostly n = 8, 10, and 12. Fig. 4a shows the correlated boson ground state when $R^{(0)+} = Q^{(0)+}$. This is the first example of the general complementarity mentioned in section 4. The state vector is more concentrated in m, at the expense of a greater spread to the first and second exact excited-states. Fig. 4b shows the

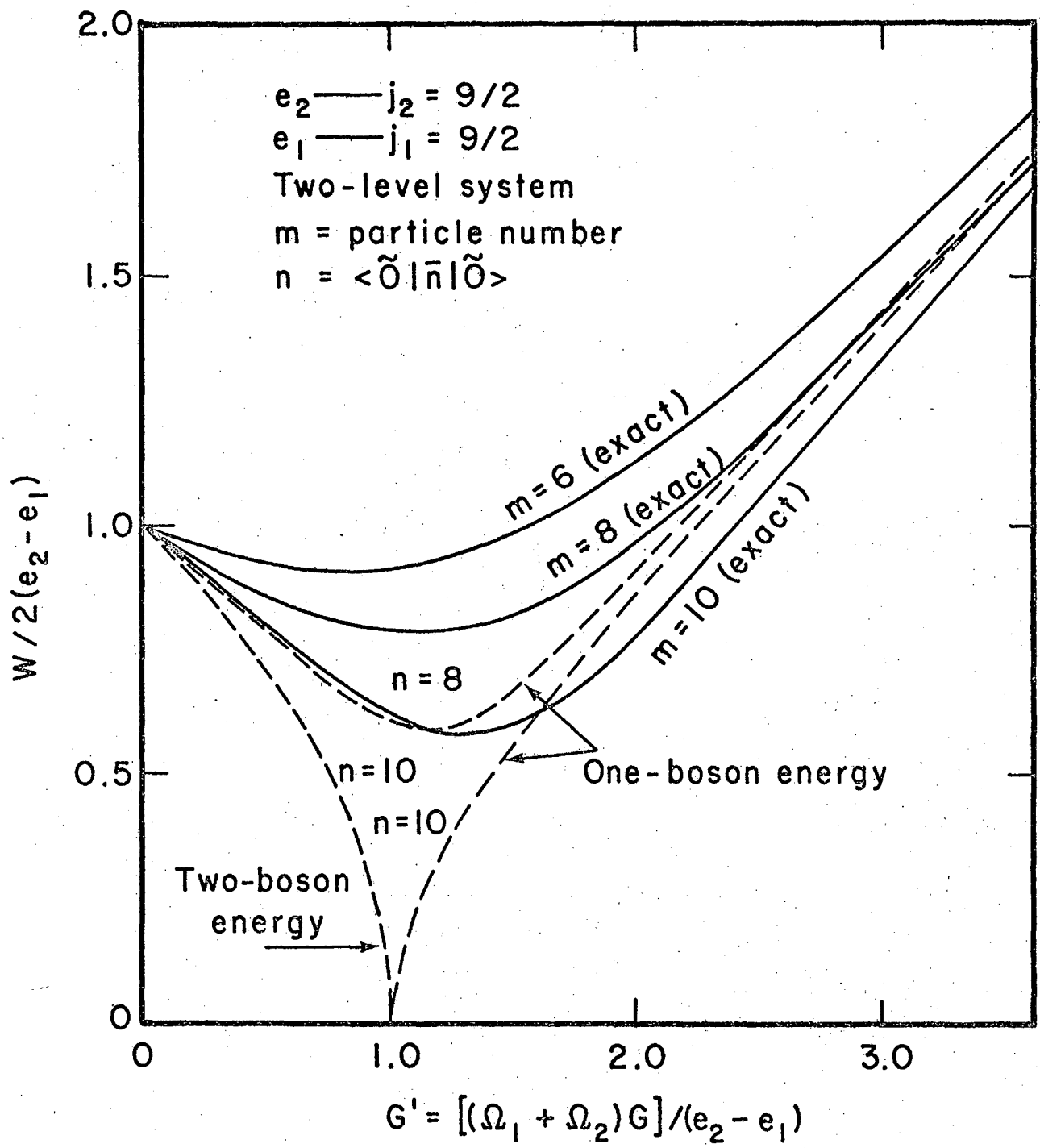

Fig. 2

Fig. 2. Boson and exact energies compared for a two level system.

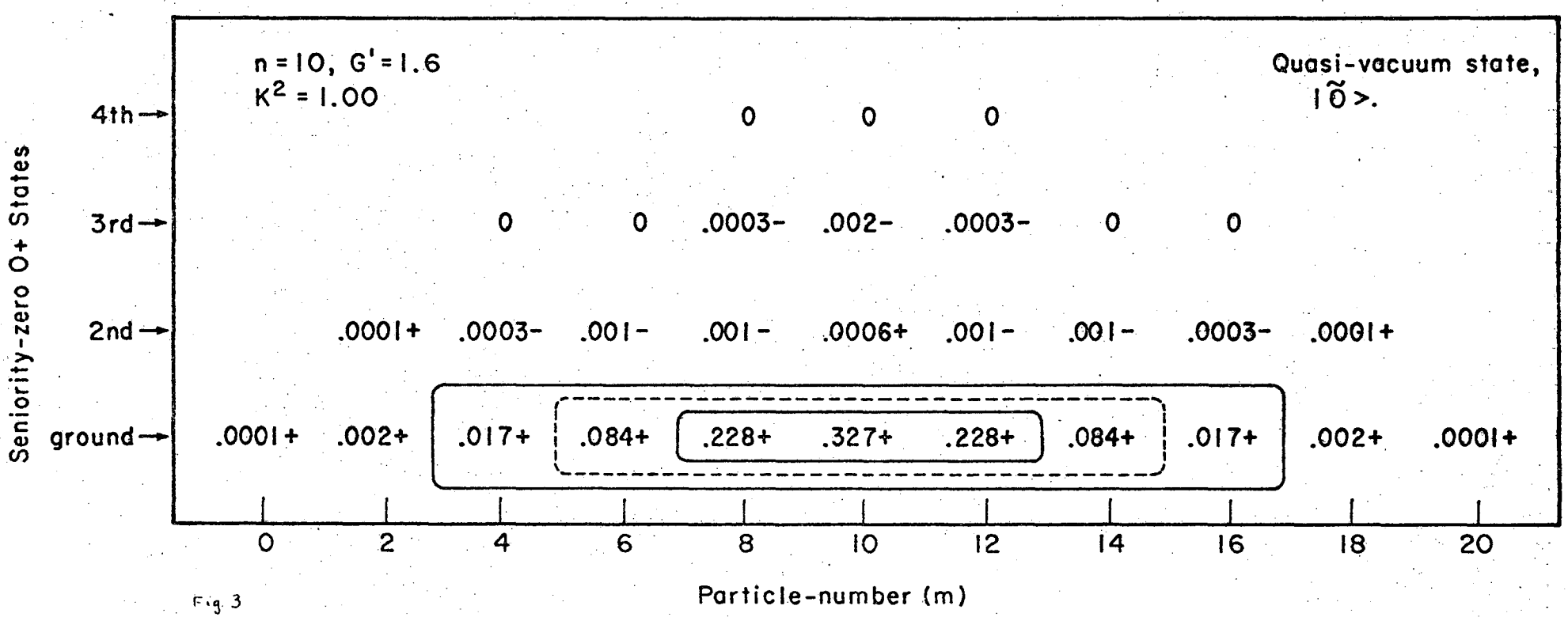

Fig. 3

Fig. 3. For a system of two j = 9/2 levels, the entries show the squared amplitudes (and signs) of projections of the quasi-vacuum state onto exact states. The average particle number, n, is 10. Potential strength, G', is 1.6.

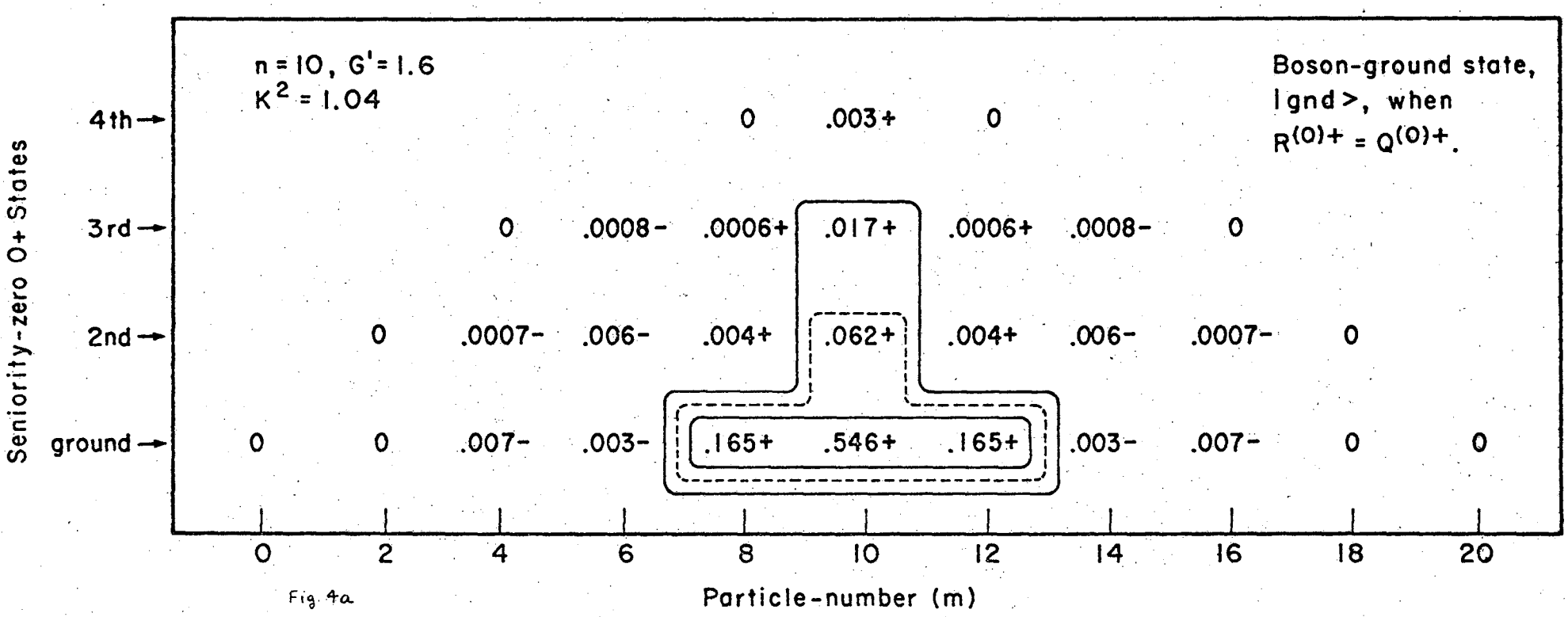

Fig. 4a. For a system of two $j = 9/2$ levels, the entries show the squared amplitudes (and signs) of projections of the quasi-boson ground state onto exact states, when the zero energy boson, $R^{(0)+}$, is chosen to be $Q^{(0)+}$: The average quasi-vacuum particle number, n, is 10. Potential strength, G', is 1.6.

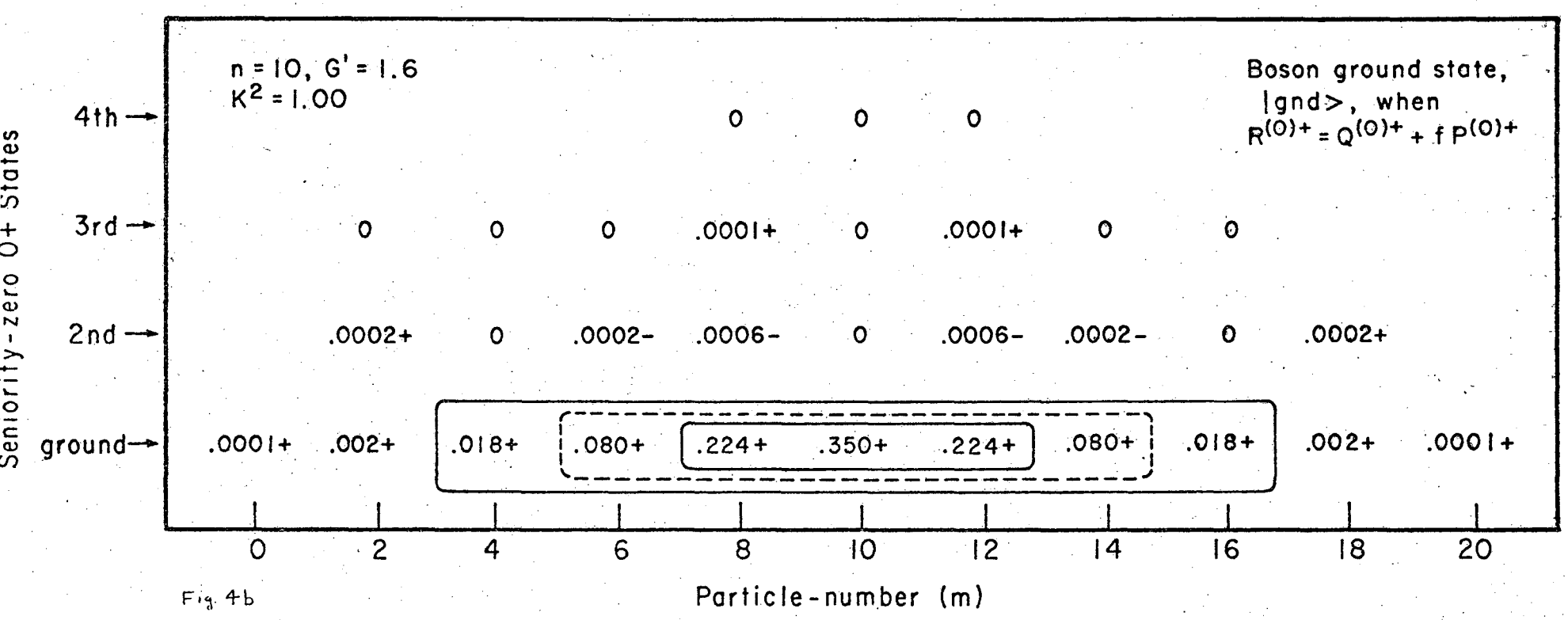

Fig. 4b

Fig. 4b. Same as fig. 4a but with zero energy boson, $R^{(0)+}$, chosen to be $Q^{(0)+} + f\ P^{(0)+}$.

correlated <u>boson</u> ground state when $R^{(0)+} = Q^{(0)+} + f\ P^{(0)+}$ (see eqs. (31) and (39)). It is slightly more concentrated in both m and energy than fig. 3. For curiosity, fig. 5 shows the correlated boson ground state when $R^{(0)+} = P^{(0)+}$. It is seen that <u>all</u> particle numbers are about equally probable. This result is not surprising if one recalls that $P^{(0)+}$ takes $|\tilde{0}\rangle$ at n into $|\tilde{0}\rangle'$ at n + dn. (See eq. (44) and discussion there.) The system makes itself insensitive to changes in n by spreading equally over all possible particle numbers.

It is possible to consider fig. 4b as a compromise between fig. 4a and fig. 5.

7.5 STATES OF ONE NON-ZERO BOSON - Figs. 6a through 8a display states of one non-zero boson for n = 10 and various G' values, in the case when $R^{(0)+} = Q^{(0)+}$. Figs. 6b through 8b do the same for the case when $R^{(0)+} = Q^{(0)+} + f\ P^{(0)+}$. It is seen that the latter figures are less spread to ground and second-excited exact states but are more spread in particle number. This behaviour shows again the complementarity seen in the ground states. For G' = 1.2 (figs. 8), both choices of $R^{(0)+}$ give a one-boson state well spread over ground and first-excited exact states, although the fig. 8b still exhibits smaller components of second and third excited exact states. Thus figs. 8 show, as does fig. 2 for the energies, the failure of the quasi-boson method for G' near unity and n equal to a shell closure.

Figs. 9 and 10 show the states of one non-zero-energy boson for the same two choices of $R^{(0)+}$, but with average particle number n = 8.

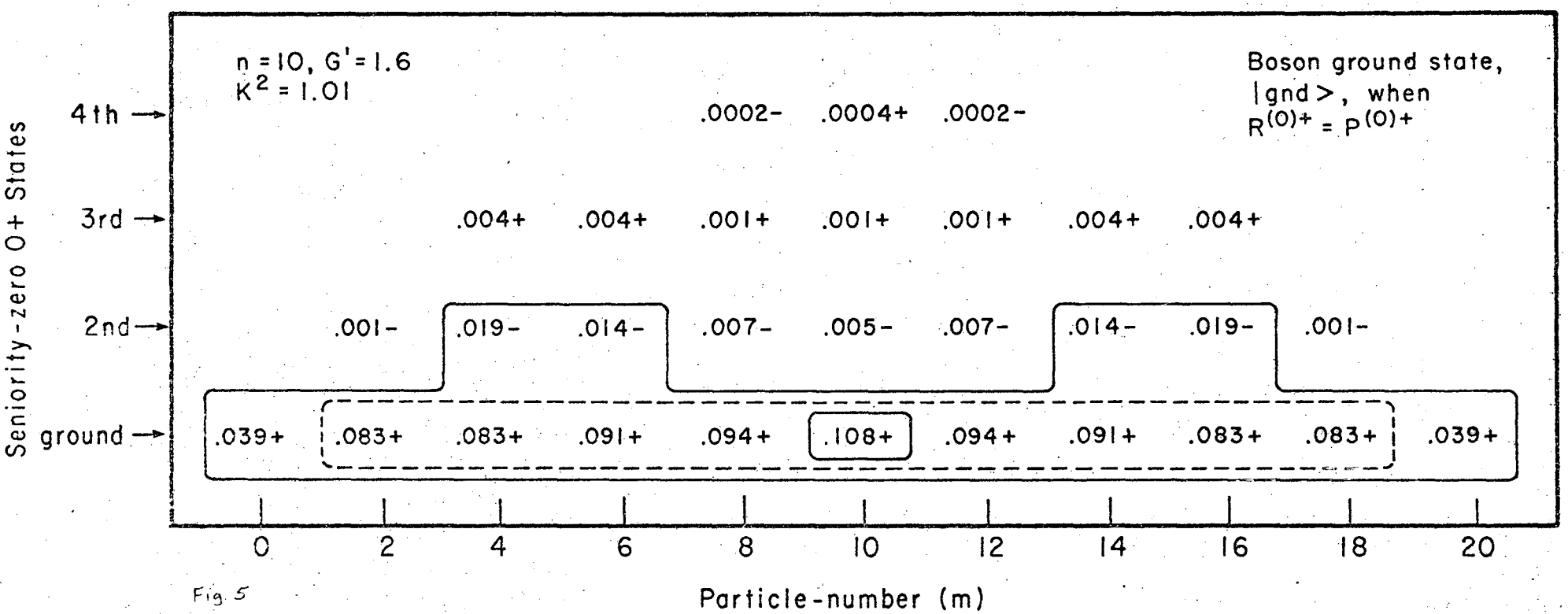

Fig. 5

Fig. 5. For a system of two j = 9/2 levels, the entries show the squared amplitudes (and signs) of projections of the quasi-boson ground state onto exact states, when the zero energy boson, $R^{(0)+}$, is chosen to be $P^{(0)+}$. The average quasi-vacuum particle number, n, is 10. Potential strength, G', is 1.6.

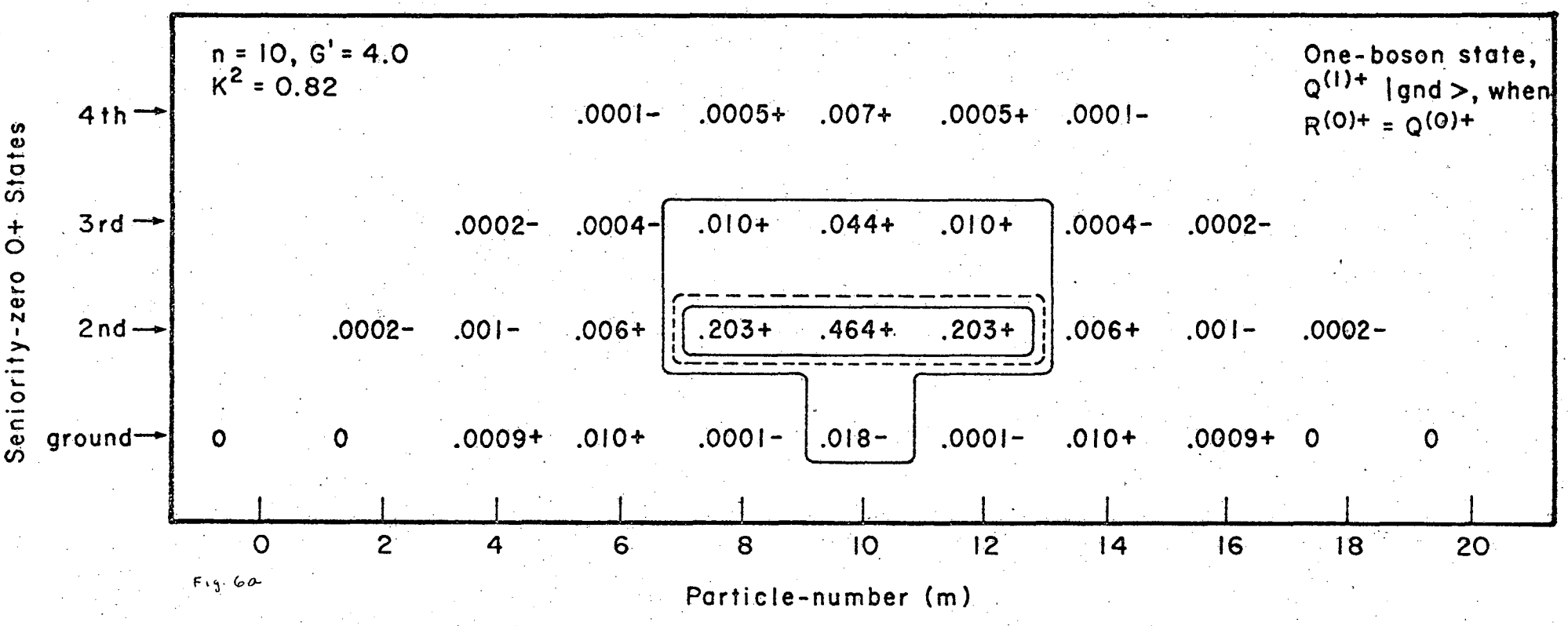

Fig. 6a

Fig. 6a. For a system of two $j = 9/2$ levels, the entries show the squared amplitudes (and signs) of projections of the non-zero energy boson state onto exact states, when the zero energy boson, $R^{(0)+}$, is chosen to be $Q^{(0)+}$. The average quasi-vacuum particle number, n, is 10. The potential strength, G', is 4.0.

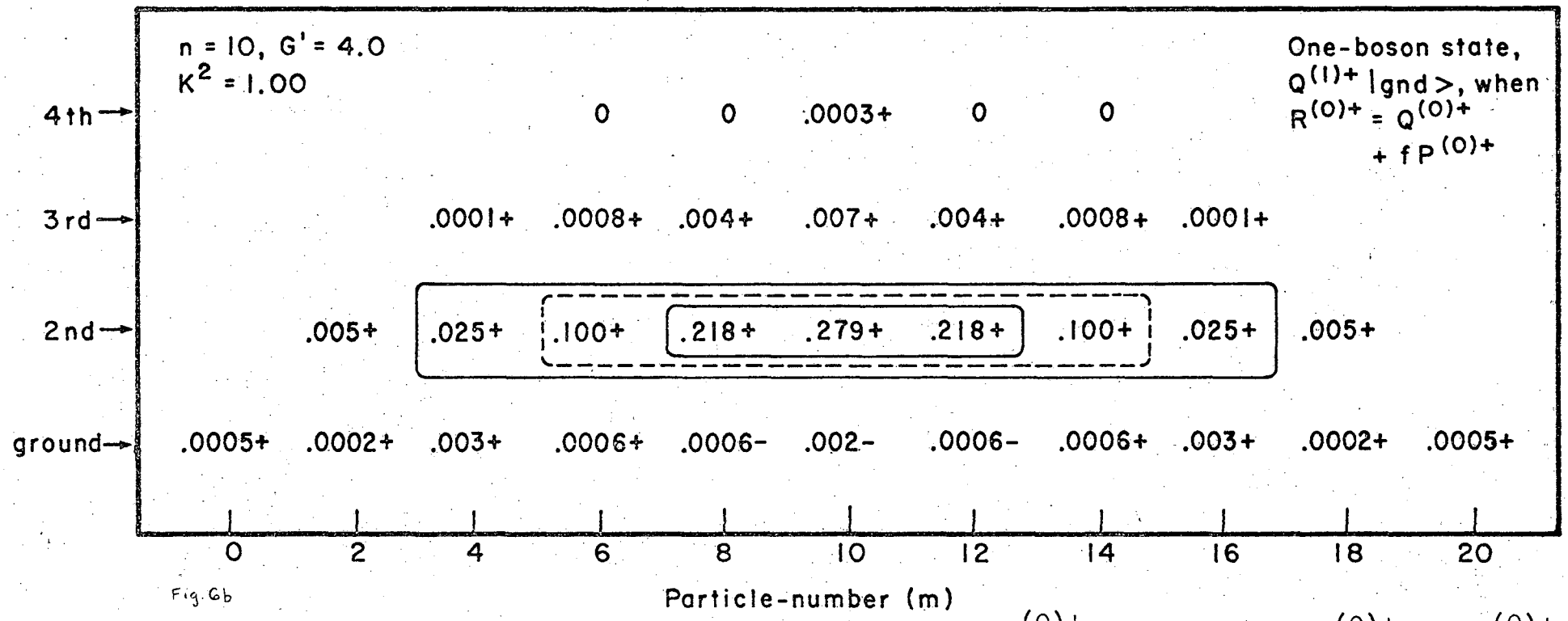

Fig. 6b

Fig. 6b. Same as fig. 6a but with zero energy boson, $R^{(0)+}$, chosen to be $Q^{(0)+} + f\,P^{(0)+}$.

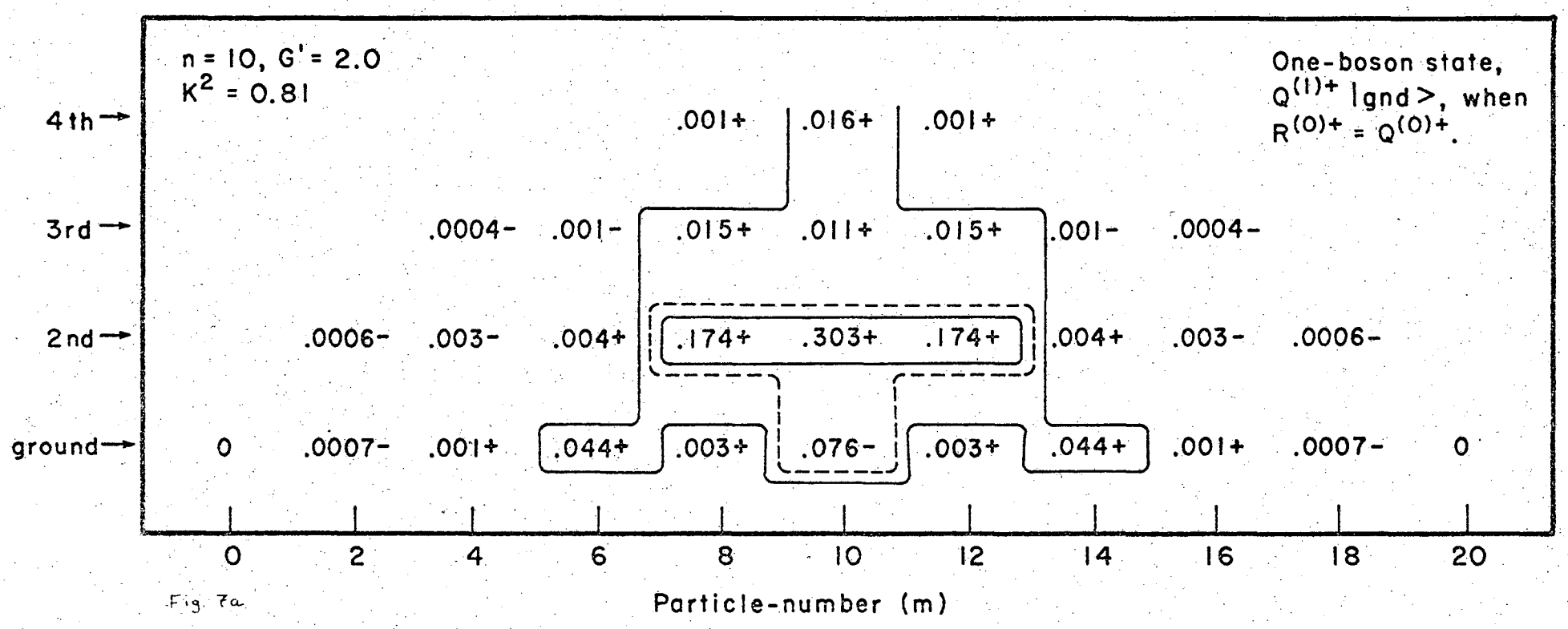

Fig. 7a

Fig. 7a. Same as fig. 6a but with potential strength, G', equal to 2.0.

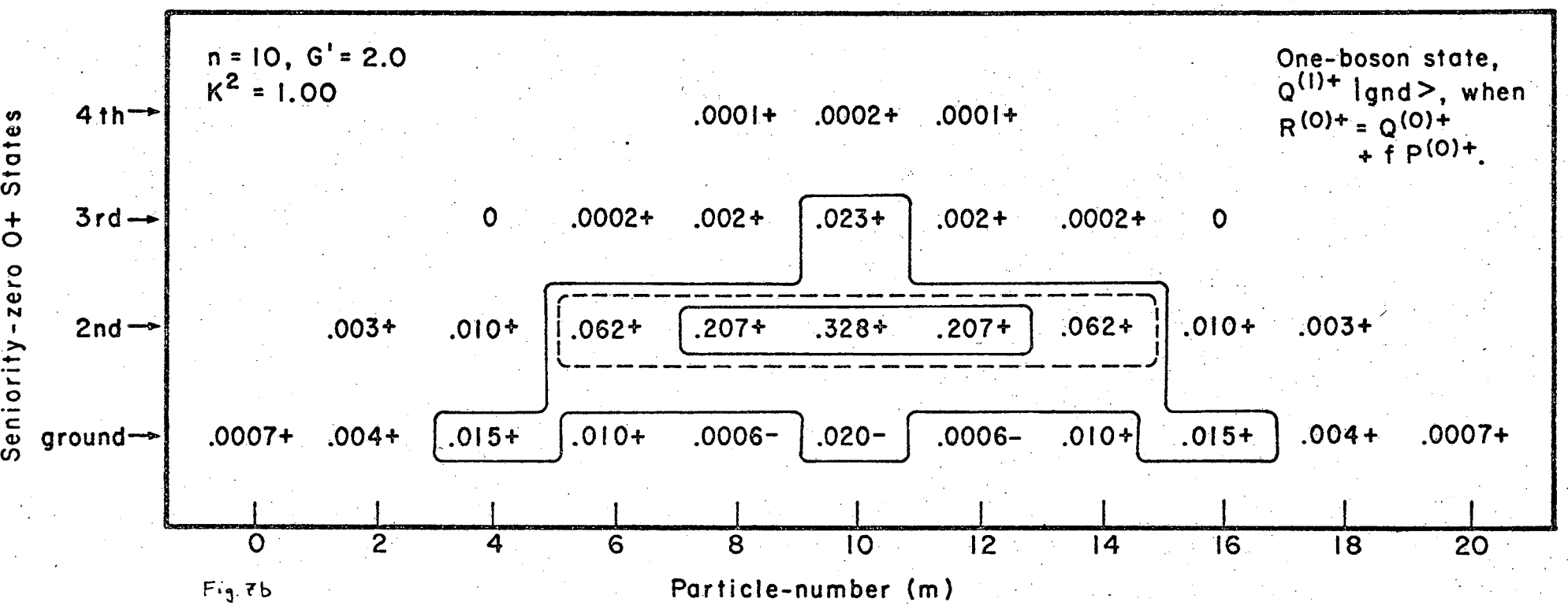

Fig. 7b. Same as fig. 6b but with the force strength, G', equal to 2.0.

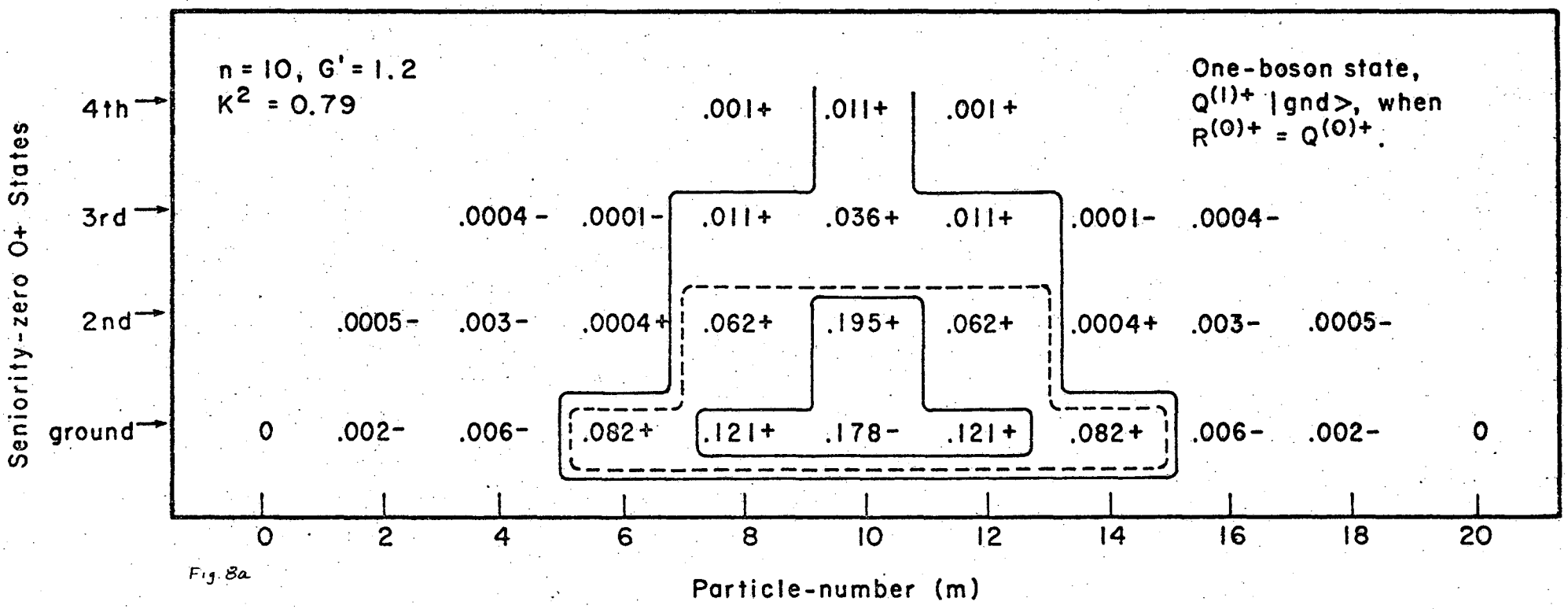

Fig. 8a. Same as fig. 6a but with the force strength, G', equal to 1.2.

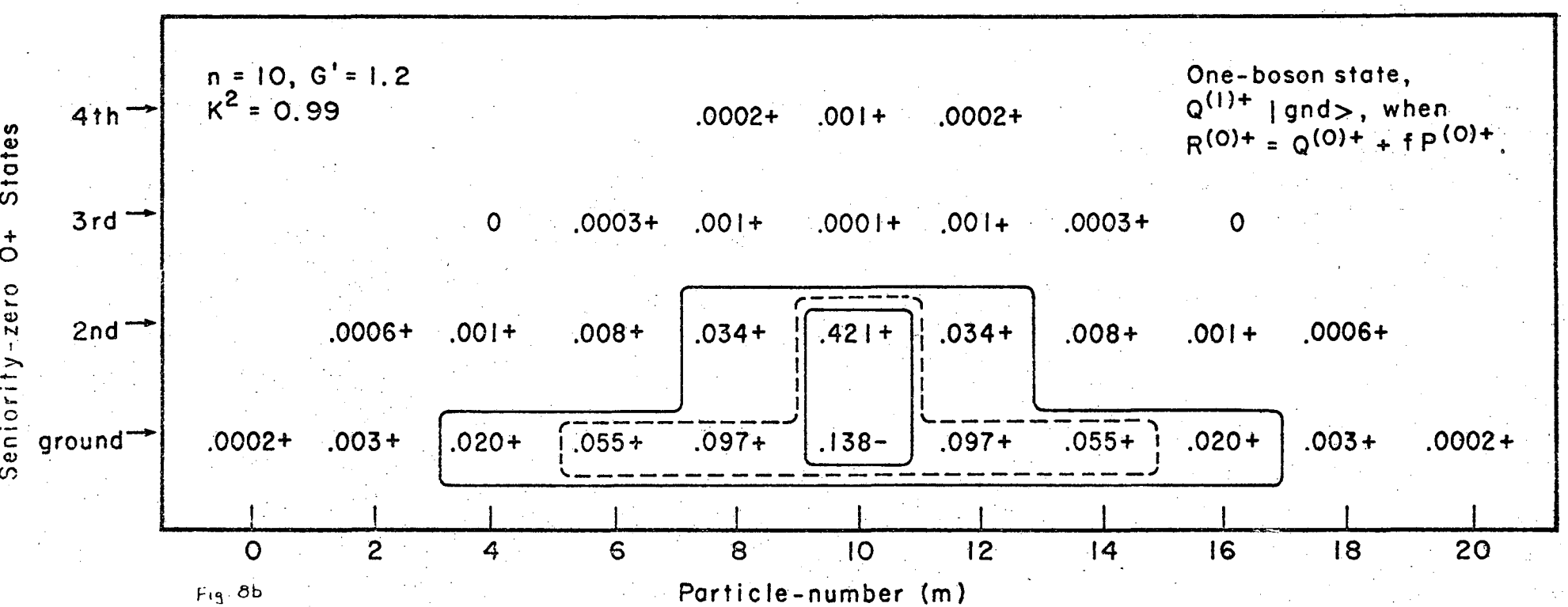

Fig. 8b. Same as fig. 6b but with the potential strength, G', equal to 1.2.

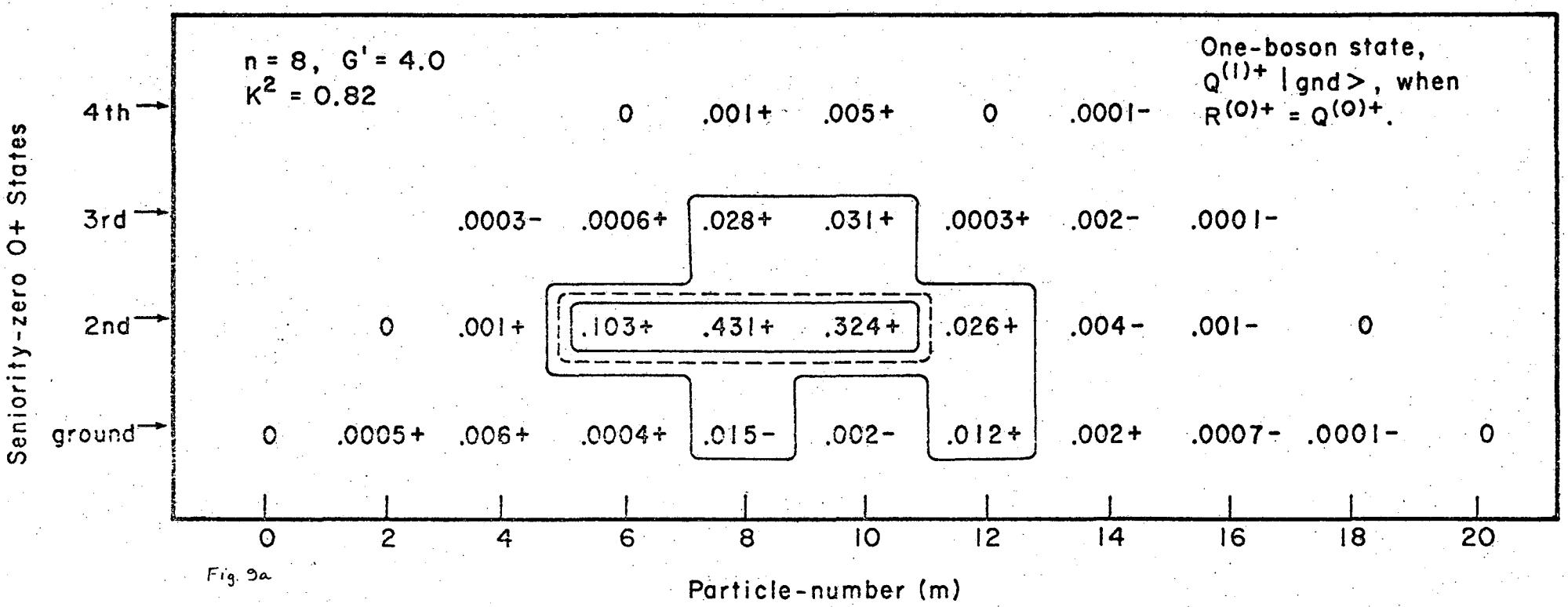

Fig. 9a

Fig. 9a. For a system of two $j = 9/2$ levels, the entries show the squared amplitudes (and signs) of projections of the non-zero energy boson state onto exact states, when the zero energy boson, $R^{(0)+}$, is chosen to be $Q^{(0)+}$. The average quasi-vacuum particle number, n, is 8. The potential strength, G', is 4.0.

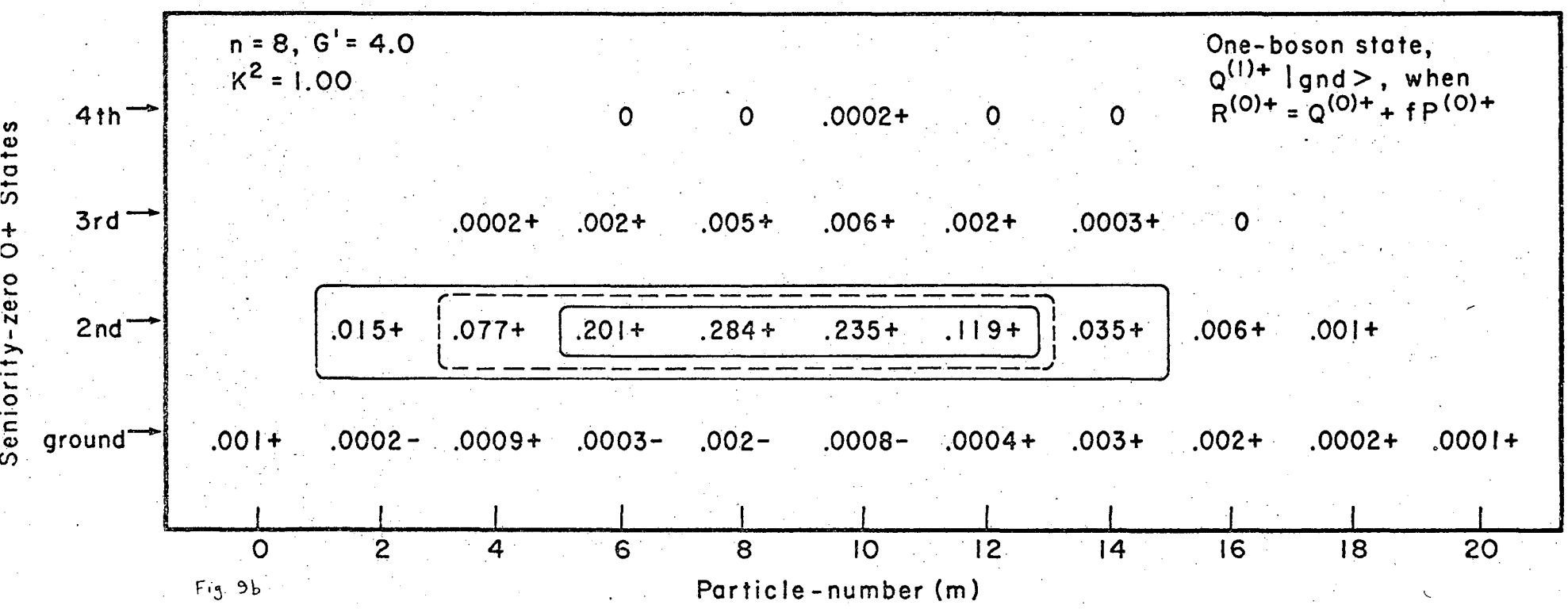

Fig. 9b

Fig. 9b. Same as fig. 9a but with zero energy boson, $R^{(0)+}$, chosen to be $Q^{(0)+} + f\,P^{(0)+}$.

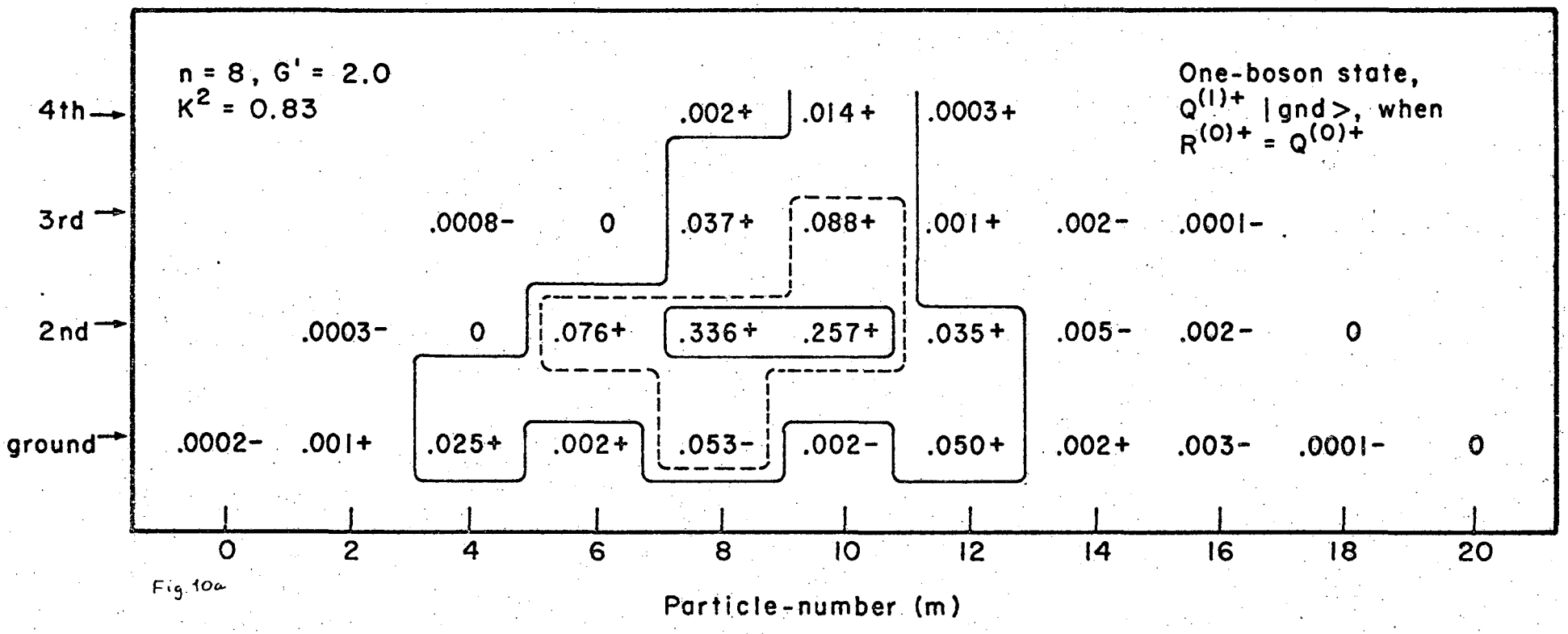

Fig. 10a. Same as fig. 9a but with potential strength, G', equal to 2.0.

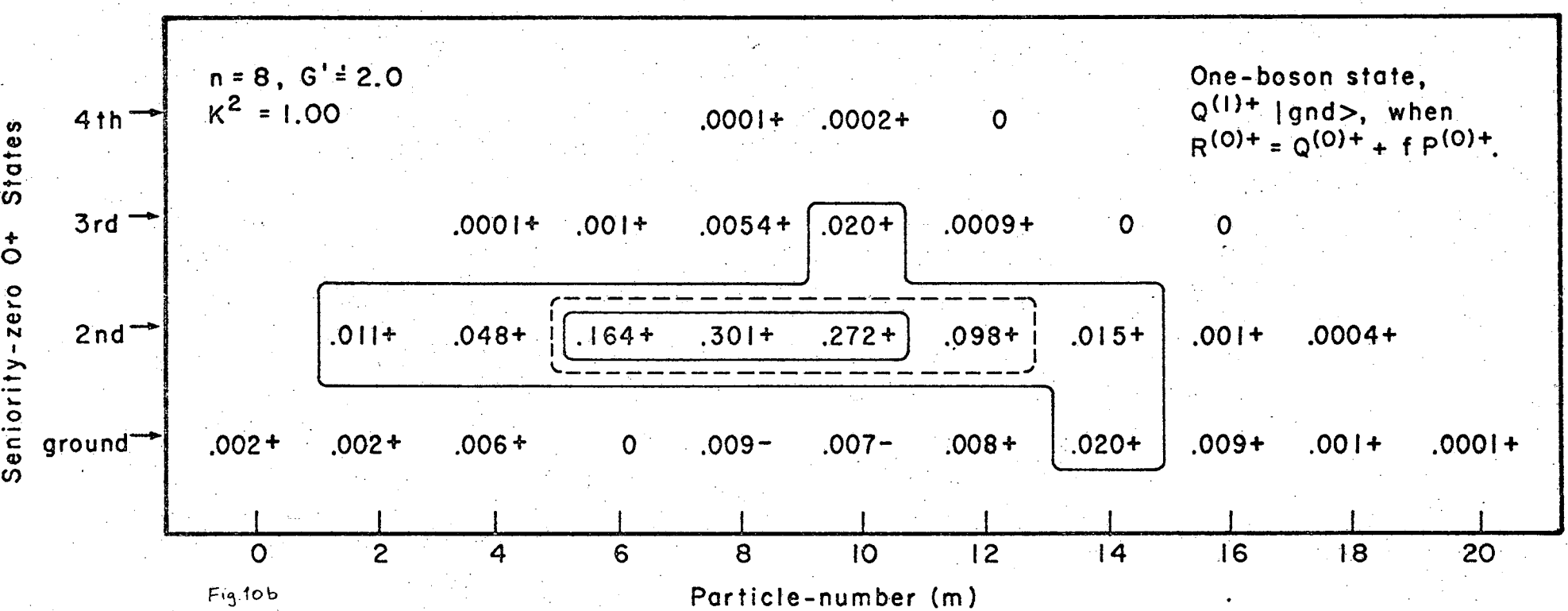

Fig. 10b. Same as fig. 9b but with potential strength, G', equal to 2.0.

The question now arises as to which choice of $R^{(0)+}$ gives the better approximation. Since the quasi-particle approximation in general is intended to be used to calculate those properties which do not change sharply as particle number is varied, it seems that a better approximation is one which, within reason, is sharper in energy and more diffuse in particle number. In this sense, the pictures (figs. 4 to 10) suggest strongly that, at least for spherical systems, and perhaps for deformed ones as well, the choice of $R^{(0)+} = Q^{(0)+} + f\ P^{(0)+}$ gives a better approximation.

7.6 STATES OF ONE ZERO-BOSON AND ONE NON-ZERO-BOSON - It is demonstrated in section 4 that $\bar{\Delta} \neq 0$, $G' \ll 1$, the <u>first</u> excited state operator should consist of one zero-boson times one non-zero-boson. This demonstration was refined in section 6 to correct an essential difficulty which occurs in all quasi-particle-type approximations in the $G' \ll 1$ limit. The result of the theory in these two sections is to predict a first excited boson state of the form, eq. (51),

$$Q^{(1)+} S^{(0)+} |gnd\rangle$$

in the $G' \ll 1$ limit of the model system when $n = 8$.

Figs. 11a,b and 12a,b show the one non-zero boson states for $G' = 1.2$ and $G' = .8$ respectively, with the two choices of $R^{(0)+}$ as before. Note that in these figures the center of the distribution in m is shifted from $m = 8$ to almost $m = 10$. This indicates that G' is small enough so that $Q^{(1)+}$ is taking on the

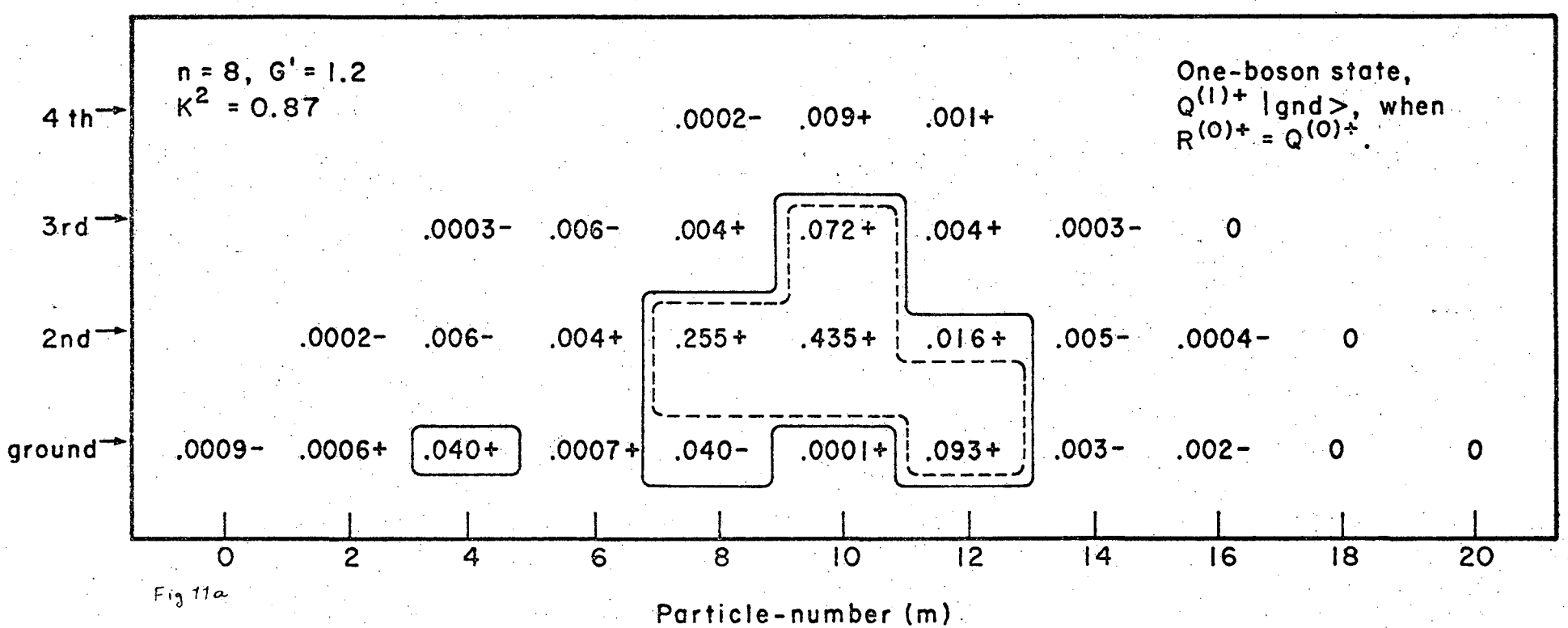

Fig. 11a. Same as fig. 9a but with potential strength, G', equal to 1.2.

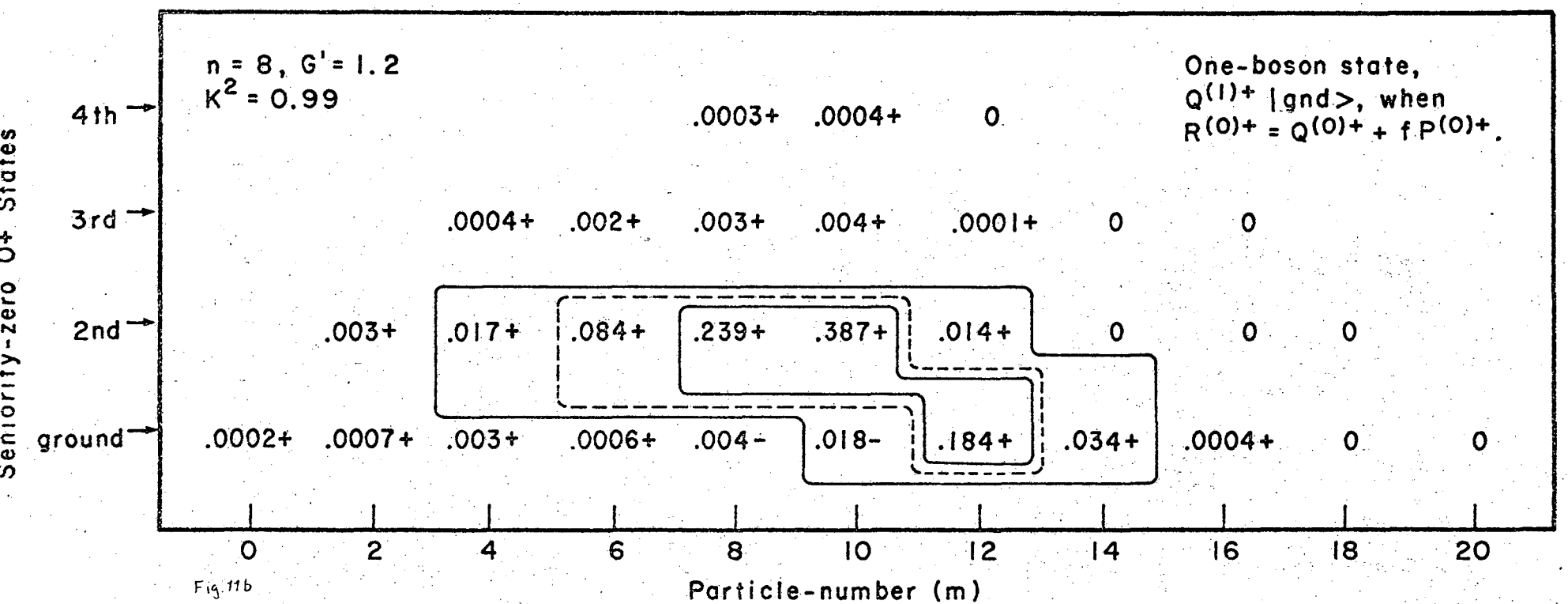

Fig. 11b. Same as fig. 9b but with force strength, G', equal to 1.2.

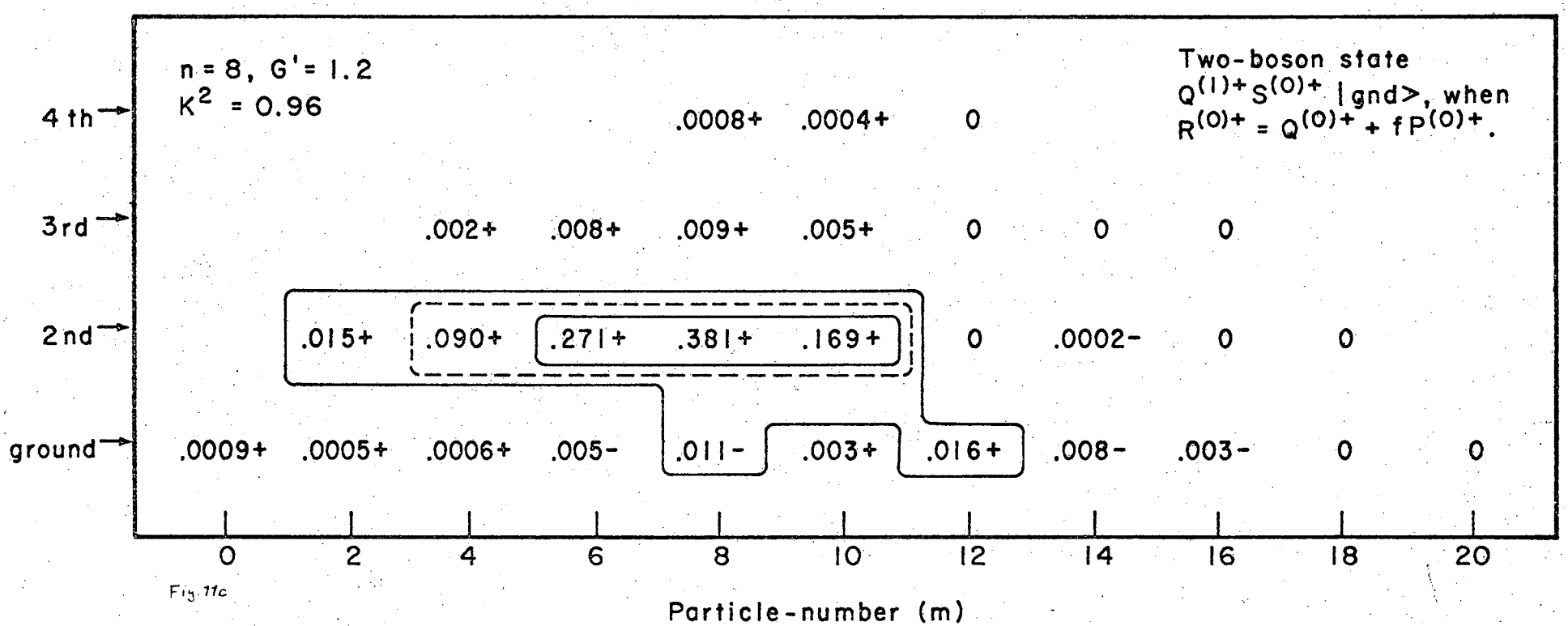

Fig. 11c. For the same system, average particle number, and potential strength as figs. 11a and 11b, the entries show the exact state projections of a two boson state consisting of one non-zero energy boson and one modified zero energy boson, $S^{(0)+}$.

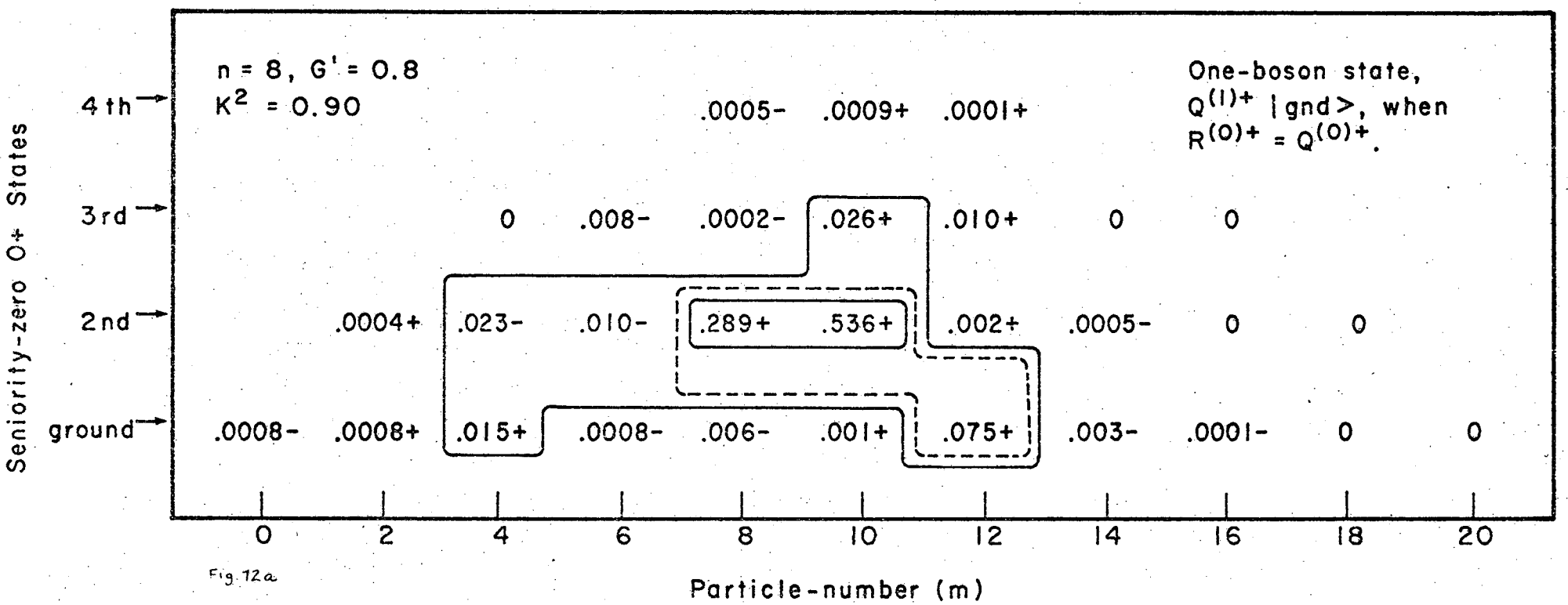

Fig. 12a. Same as fig. 9a but with potential strength, G', equal to 0.8.

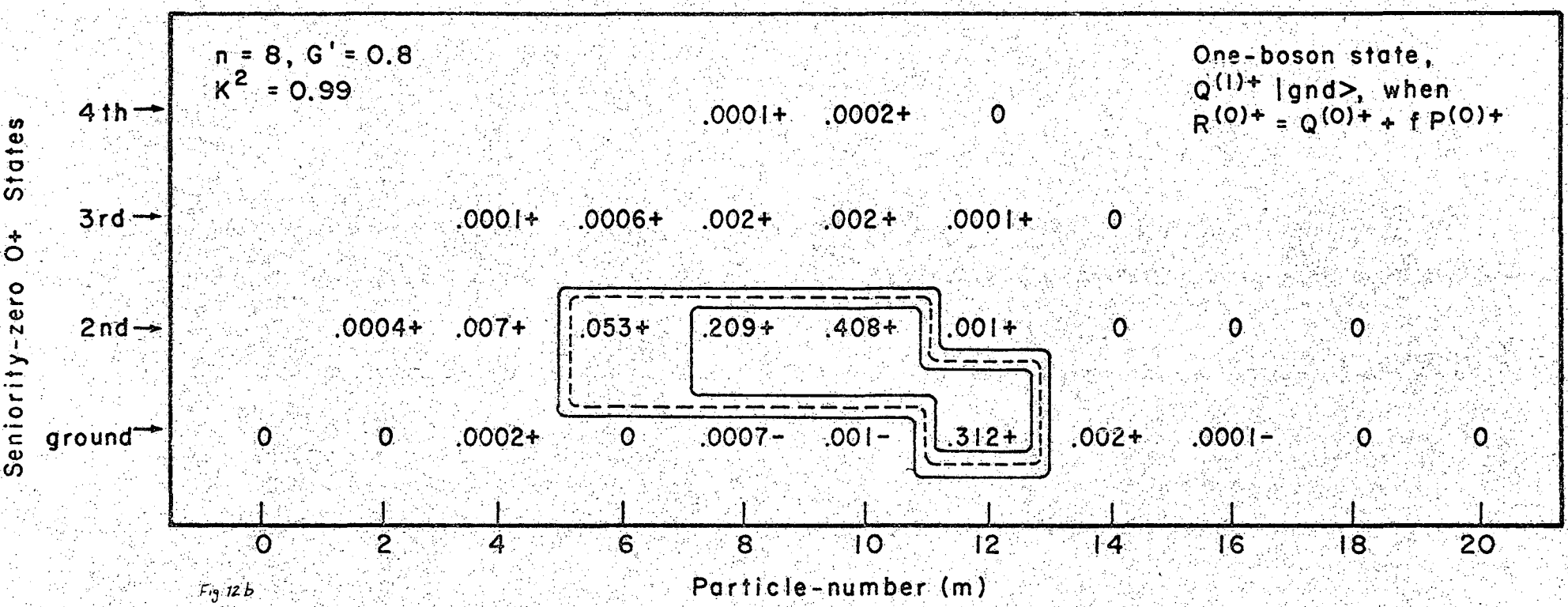

Fig. 12b. Same as fig 9b but with force strength, G', equal to 0.8.

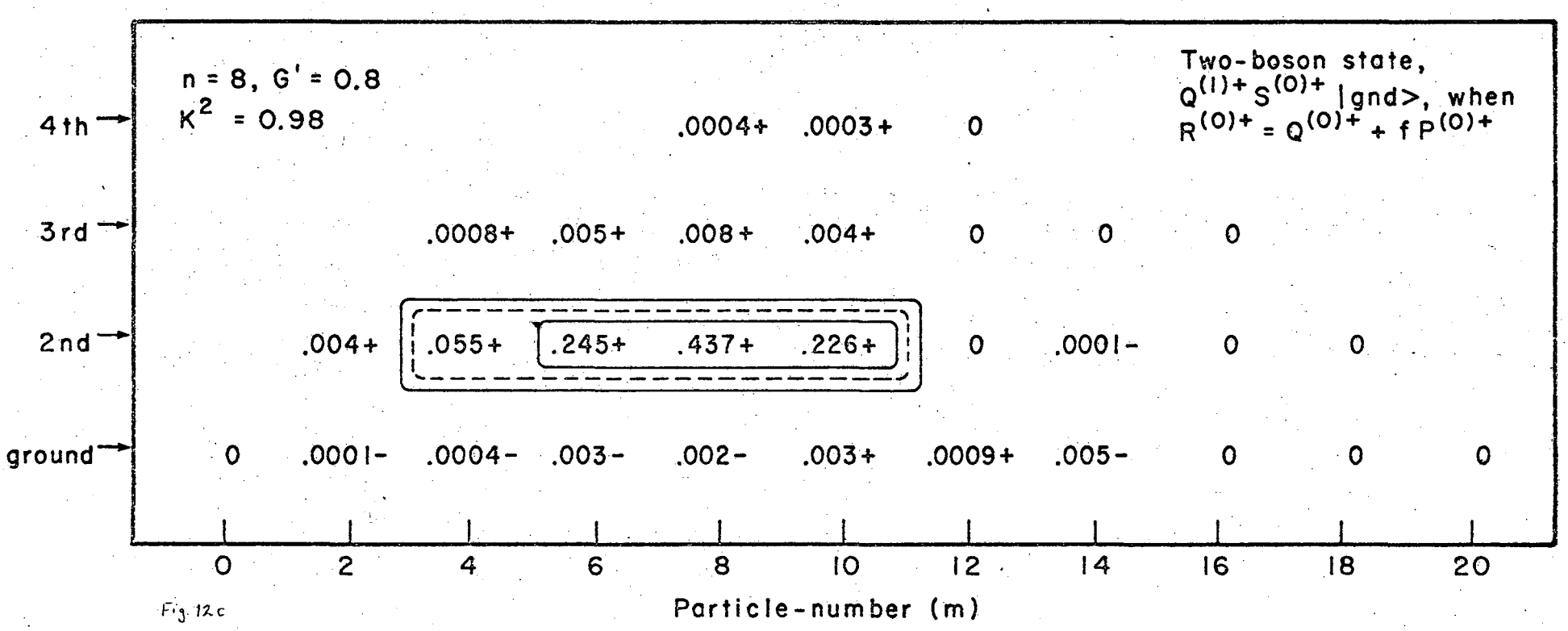

Fig. 12c

Fig. 12c. For the same system, average particle number, and potential strength as figs. 12a and 12b, the entries show the exact state projections of a two boson state consisting of one non-zero energy boson and one modified zero energy boson, $S^{(0)+}$.

character of a two-real-particle creation operator. In figs. 11c and 12c the boson $S^{(0)+}$ has been multiplied into the states of figs. 11b and 12b. The number distribution now centers on m = 8, and the spread to the ground state of the m = 6 system is much reduced. These figures corroborate the arguments of section 4 that for $G' < 1.2$, $\bar{\Delta} \neq 0$, the first excited state is indeed a two boson state.

7.7 THE DEGENERATE CASE - ($\bar{\Delta} = 0$, $G' \neq 0$) - When n = 10, and $G' < 1$, the model system has $\bar{\Delta} = 0$. In this case, secular equation, eq. (17), replaces eq. (14), and the model has two non-zero roots (and no zero roots). Fig. 13a shows the vacuum state for G' = 0.8. This is just the shell model state with ten particles in level-one and no mixing of configurations. Fig. 13b shows the correlated boson-ground state. The correlations introduced by the bosons give a striking improvement over fig. 13a. Fig. 13c shows the two-non-zero-boson state. (The one-non-zero-boson states are pure m = 8 or m = 12 states.)

Comparison of fig. 8b (G' = 1.2, n = 10) with fig. 11c (G' = 1.2, n = 8) and comparison of fig. 13c (G' = 0.8, n = 10) with fig. 12c (G' = 0.8, n = 8) will show that, at least for excited states, the failure of the quasi-boson method for n = 10, G' around unity, is bad enough that one would expect the properties of the m = 10 exact system to be better represented by n = 8 than by n = 10. This is more evidence for the rule-of-thumb mentioned in sub-section 7.3 when discussing boson energies.

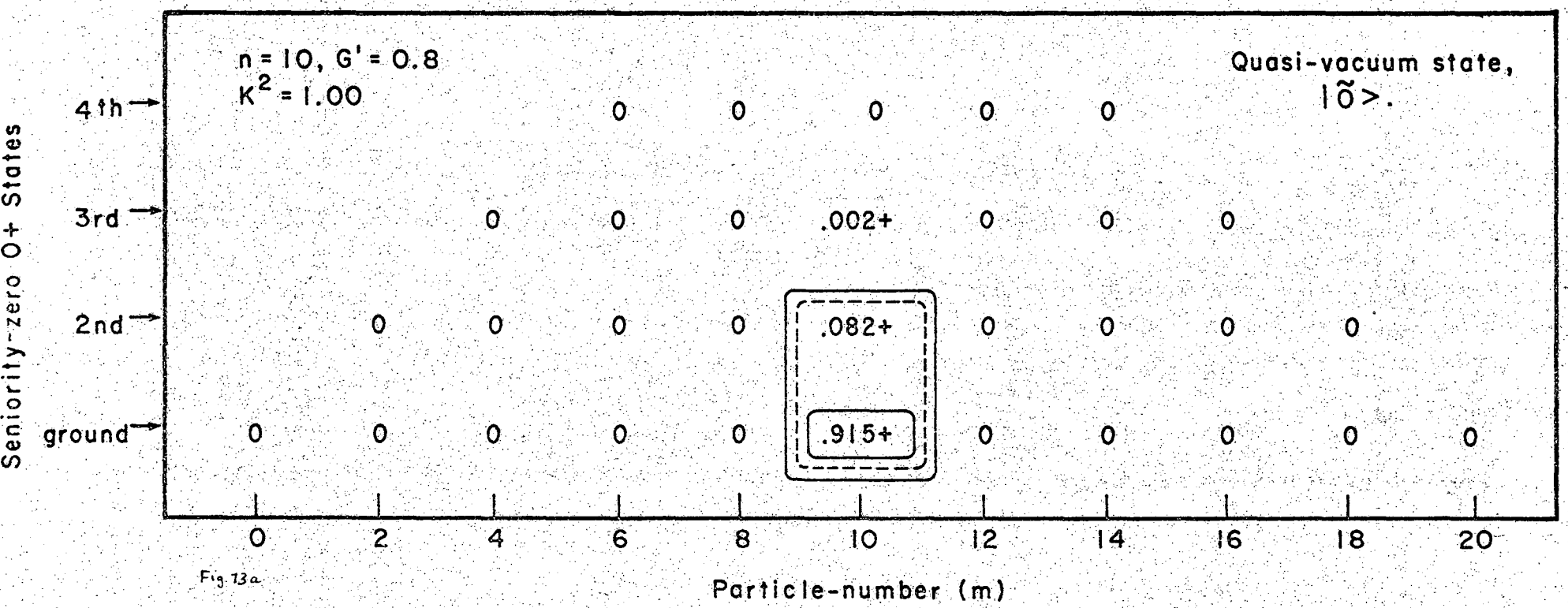

Fig. 13a

Fig. 13a. For a system of two j = 9/2 levels, the entries show the squared amplitudes (and signs) of exact state projections of the quasi-vacuum state (degenerate state). The particle number is 10. The potential strength, G', is 0.8.

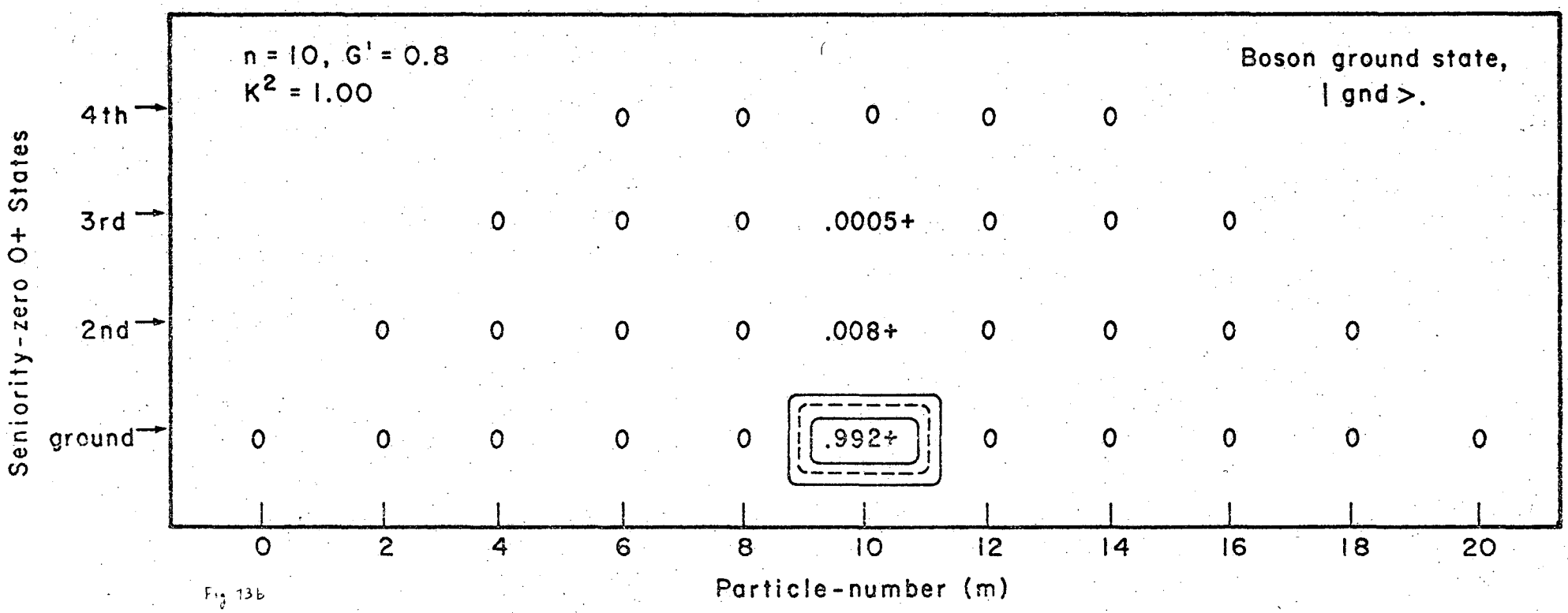

Fig. 13b. For a system of two j = 9/2 levels, the entries show the squared amplitudes (and signs) of exact state projections of the boson ground state. The particle number is 10. The force strength, G', is 0.8.

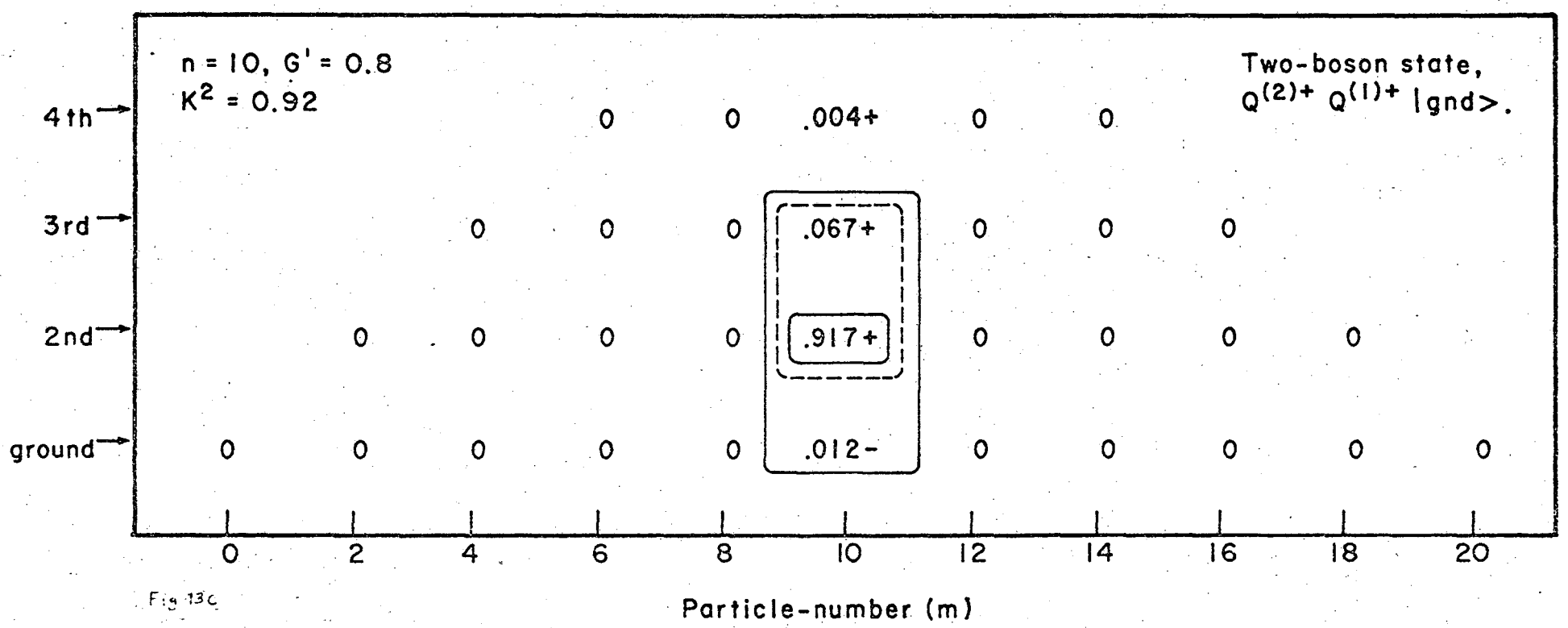

Fig. 13c

Fig. 13c. For a system of two $j = 9/2$ levels, the entries show the squared amplitudes (and signs) of exact state projections of the state of the two non-zero energy bosons. The particle number is 10. The potential strength, G', is 0.8.

7.8 THE TWO NON-ZERO-BOSON STATE - Fig. 14 displays the state of two non-zero bosons, for G' = 2 and n = 10. Comparison with fig. 7b shows that the two-boson state is much more spread in energy over the various exact excited states than was the one non-zero boson state at the same G' and n.

7.9 THE PRIMITIVE PAIR-VIBRATION STATE - Fig. 15 shows the state derived in eq. (45), and called the primitive pair vibration, for reasons given there. This state turns out to be almost identical to the two-boson state above. (Compare figs. 14 and 15.) This result, which is also found at other n and G' values (not shown in figure), is discussed in section 5.

7.10 MAGNITUDE OF FORCE-STRENGTH - To generalize the numerical results of this section to more complex systems, such as actual spherical or deformed nuclei, it is necessary to know which force strength, G', of the present model system corresponds to the force strengths used in the complex systems.

The failure of the quasi-boson method at the closed-shell (n = 10 in the model system) occurs in the vicinity of the critical G value, G_c. (G' = 1) This suggests that a useful parameter for comparison of various systems will be the ratio of G for each system to G_c for that system. This parameter

$$G' = \frac{G}{G_c} \tag{53}$$

tells how strong the force is in a given system compared to the force at which the approximation fails for that system. The

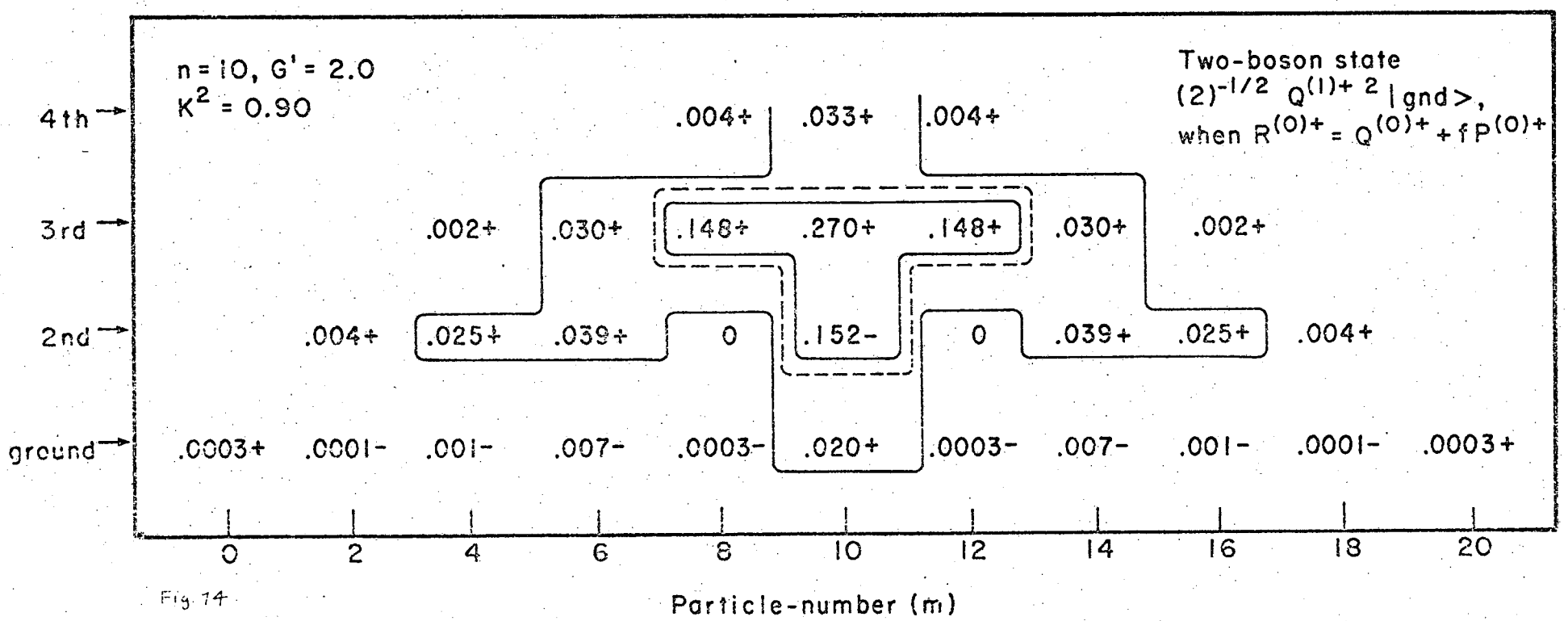

Fig. 14

Fig. 14. For a system of two $j = 9/2$ levels, the entries show the squared amplitudes (and signs) of projections of the two non-zero energy boson state onto exact states. The zero energy boson, $R^{(0)+}$, is chosen as shown on the figure. The average quasi-vacuum particle number, n, is 10. The potential strength, G', is 2.0.

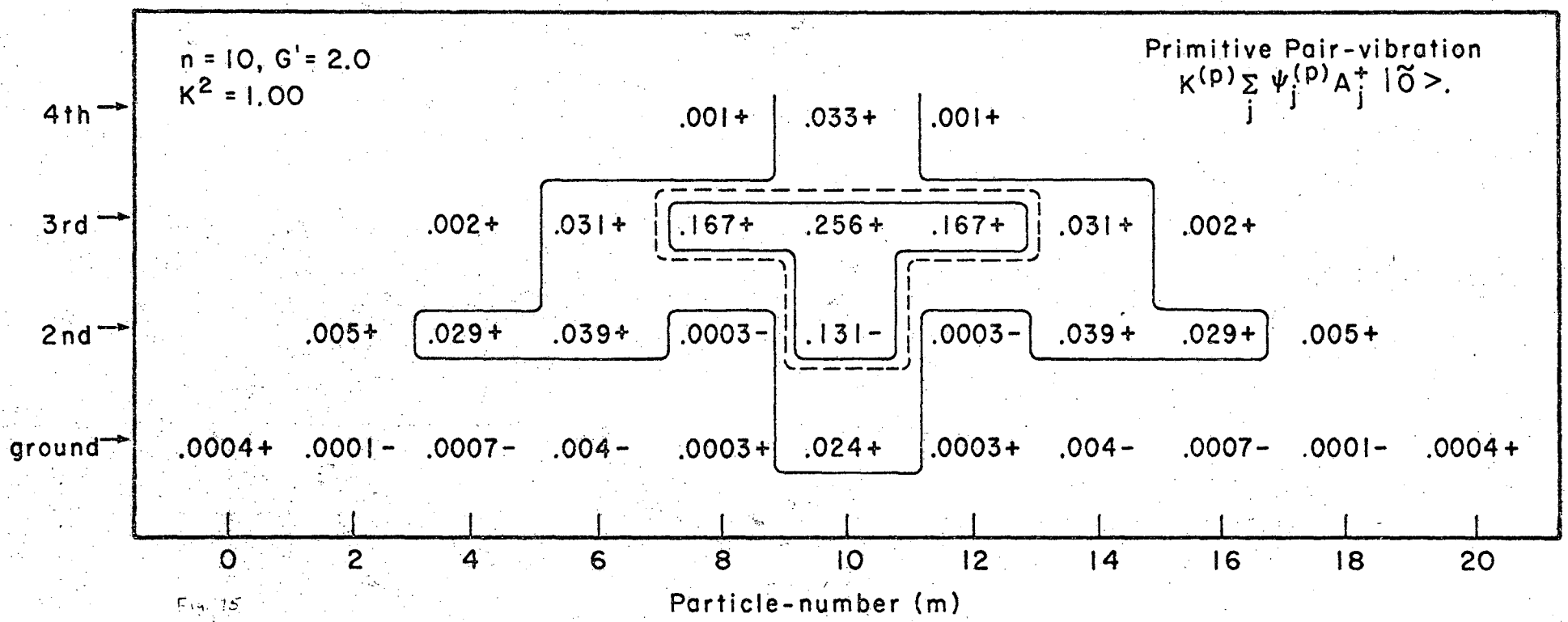

Fig. 15. For a system of two j = 9/2 levels, the entries show the squared amplitudes (and signs) of projections of the primitive pair vibration state, eq. 45, onto exact states. The average quasi-vacuum particle number, n, is 10. The potential strength, G', is 2.0.

present calculations with the two-level model system suggest that, for systems with a partially filled sub-shell, G_c should be chosen by interpolation of the critical G values at the nearest sub-shell closures. For many systems, G_c will approximate the minimum of the first excited state excitation energy versus G curve. (See, eg., fig. 2 for m = 6 and m = 8.)

For spherical systems, a useful estimate to G_c at sub-shell closures is given by

$$G_c = \frac{e_a - e_b}{\Omega_a + \Omega_b} \tag{54}$$

where "a" and "b" denote orbits just above and below the fermi-energy at the sub-shell closure. This estimate is exact for the model system described in section 7.1, and is used in eq. (52).

Fig. 16 shows $\bar{\Delta}$ versus G' for the model system (dashed lines) and for a neutron system of 36 levels in the rare-earth deformed region. The latter system is that used in a published calculation of β and γ vibrations.[†] The two systems are shown both with n at a closed shell and with n one less than a shell closure. It is seen that, eg., at G' = 1.2, the fractional difference between the two solid curves is about the same as the fractional difference between the two dashed curves. This supports the idea that G' is

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[†] Single particle levels for fig. 16 are taken from Table I of reference[3]).

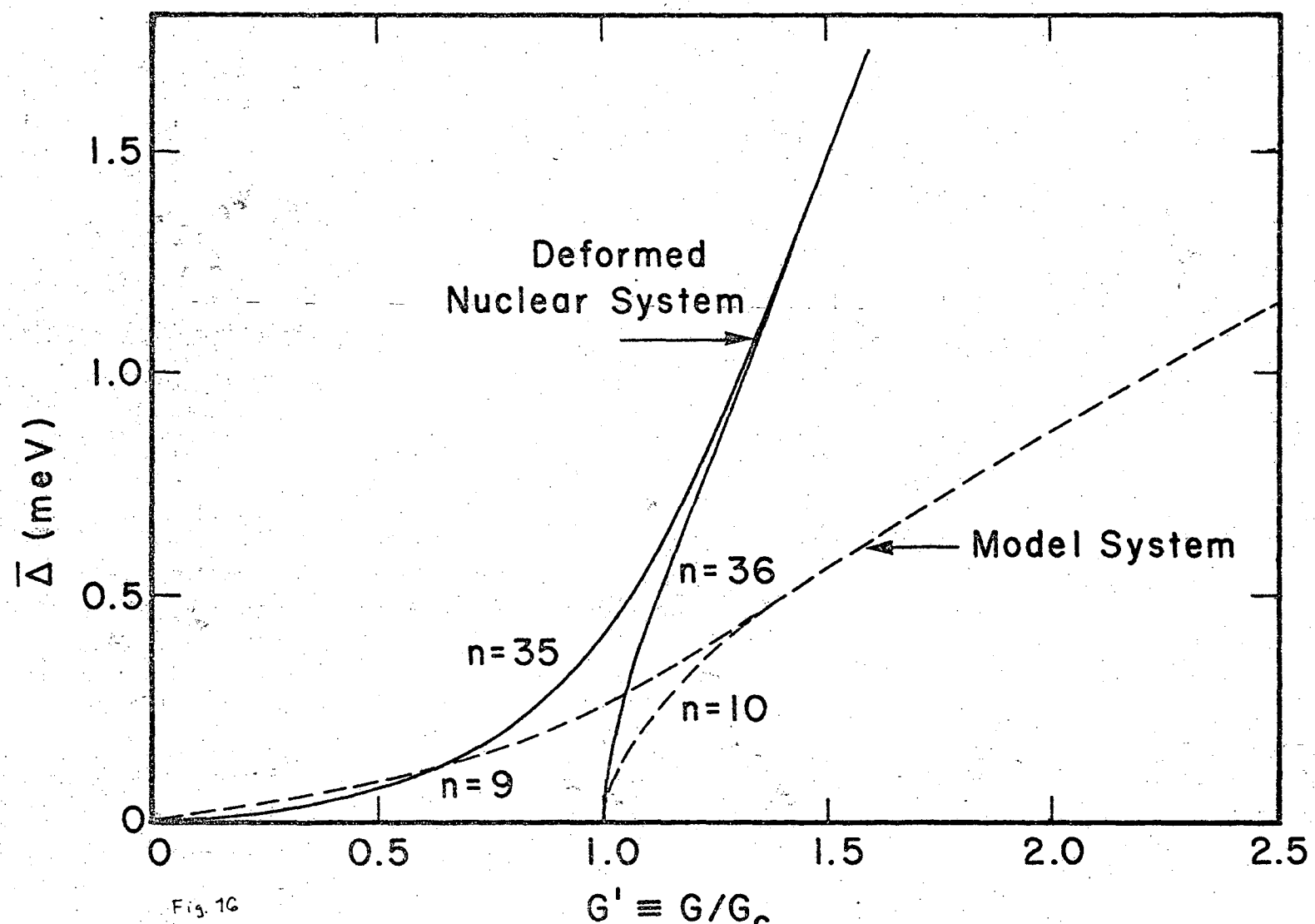

Fig. 16

Fig. 16. Plot of $\bar{\Delta}$ versus G' for the deformed system cited in the text and for a model system of two j = 9/2 levels with $(e_2 - e_1)$ = 1.0 MeV.

a useful parameter for comparison. Examination of figs. 8 showing the one-boson state for n = 10, G' = 1.2 shows that the boson approximation is beginning to fail badly at that force strength with n at a closed subshell. The force strength used in the cited paper[3]) seems to correspond to about G' = 1.23. In fact the author[3]) notes that he obtained better results in some cases by replacing the equivalent of the last of eqs. (4),

$$n = \langle \tilde{0} | \bar{n} | \tilde{0} \rangle$$

by

$$n = \langle gnd | Q^{(k)} \bar{n} Q^{(k)+} | gnd \rangle .$$

It is possible that this replacement may have the same effect as a slight change in n. It is worth noting, also, that at G' = 1.2 the present model system predicts a <u>two</u> boson first excited state. (One zero-energy-boson times one non-zero-energy boson.) However, the great differences between the present model system and the system[3]) make direct comparison of results difficult.

A more direct comparison can be made with published calculations in spherical nuclei[6,7]). In ref.[7]) the quasi-particle TDA method is used with a surface-delta force. The authors compare the energy levels with experiments and with exactly calculated values. Some G' values used in their calculations (taken from Table 1 of [7]), using eqs. (53) and (54) of the present paper) are shown in Table 1. The values shown are at closed subshells and should be interpolated between them as noted above.

Table 1

Nucleus	G	G_c	G'
Ni^{60}	0.48	0.16	3.0
Sn^{114}	0.23	0.2	1.1
Sn^{116}	0.23	0.14	1.6
Pb^{206}	0.15	0.14	1.1
Pb^{200}	0.14	0.07	2.0
Ce^{140}	0.20	0.11	1.8

The force strengths at Sn^{114} and Pb^{206} are seen to be very weak. At these strengths the present calculation shows the uncorrelated quasi-particle ground state (TDA ground state) to contain more than a 4% component of first-excited-state strength (value at G' = 1.2, n = 10, figure not shown) as compared to less than 1% for the correlated boson ground state. At these same values of G' and n, the TDA one boson state has a 40% component of ground-state strength and a 3% component of 2nd-excited state strength (figure also not shown). Like the RPA (fig. 8b), at closed subshells for G' less than about 1.2 the TDA fails to predict correctly the seniority zero 0+ first excited state.

At G' = 1.2 or less, the present calculation also predicts that the correct first excited state for the partially-filled-shell case is a two boson state, one zero-energy boson and one non-zero energy boson. A similar result should be expected for the TDA method.

8. Projection of Correct Particle Number

As discussed in section 7, the quasi-particle and quasi-boson methods produce state vectors which are sums of terms with different particle number. The correct particle number can be selected from quasi-boson states by means of the projection operator

$$Z_m = \prod_{\substack{q=0 \\ q\neq m}}^{2\Omega} \frac{\bar{n}-q}{m-q} \quad .$$

The projected terms must then be renormalized. For example, in fig. 6b, projection of the m = 10 terms from the one boson state will give a state

$$Z_{10}\, Q^{(1)+} |gnd\rangle = -(0.002)^{\frac{1}{2}} |\Phi_0\rangle +$$

$$+ (0.279)^{\frac{1}{2}} |\Phi_1\rangle + (0.007)^{\frac{1}{2}} |\Phi_2\rangle + \cdots$$

where $|\Phi_k\rangle$ are the exact eigen states of the m = 10 system. After normalization, this state is

$$-(0.007)^{\frac{1}{2}} |\Phi_0\rangle + (0.968)^{\frac{1}{2}} |\Phi_1\rangle + (0.024)^{\frac{1}{2}} |\Phi_2\rangle + \cdots$$

which indicates a 97% overlap between the projected one boson state and the corresponding exact state.

Table 2 shows the overlap integrals between states

obtained by projection from the quasi-boson method and the corresponding exact states. Asterisks (*) denote the best approximations to the given exact states. The entries in parentheses refer to the original quasi-boson method[1]), with function f in eqs. (31) equal to zero. The entries no in parentheses refer to the choice of f derived in this paper, eq. (39). Note that the latter choice gives greater overlap with exact states. The overlap betwen approximate and exact states is generally better for ground states than it is for one boson states. For ground states, fig. 2 shows that methods of this paper give overlap percentages greater than 99.9% for all values of G'. The states of one quasi-particle (odd nuclei, not treated here) should have overlap percentages comparable to the ground state since they differ from the ground state only in the blocking of one pair.

For $G' \leq 1.2$ and $n = 8$, the one boson state in some cases has a slightly greater overlap than does the correct two boson state. Projection of particle number removes the components of incorrect states belonging to a different particle number.

Note also that for even a fairly strong force, $G' = 2.0$, a larger overlap integral for the $m = 10$ excited state is obtained when the average number, n, is 8 instead of 10. This suggests that calculations which are to be followed by particle number projection should perhaps always be performed with n shifted slightly from subshell closures.

Table 2

Exact State	G'	Projected Number, m	Average Number, n	Quasi-boson State	Overlap (%)	Figure Reference
gnd.	4.0	10	10	$\|gnd\rangle$	100* (98)	
gnd.	2.0	10	10	$\|gnd\rangle$	100* (91)	
gnd.	1.6	10	10	$\|gnd\rangle$	100* (87)	Fig. 4b (4a)
gnd.	1.6	10	10	$\|\mathcal{D}\rangle$	99.2	Fig. 3
gnd.	1.2	10	10	$\|gnd\rangle$	98 (86)	
gnd.	1.2	10	8	$\|gnd\rangle$	100* (90)	
gnd.	0.8	10	8	$\|gnd\rangle$	100* (98)	
gnd.	0.8	10	8	$\|\mathcal{D}\rangle$	99.9	
gnd.	1.2	8	8	$\|gnd\rangle$	99.9* (94)	
gnd.	0.8	8	8	$\|gnd\rangle$	99.9*	
gnd.	0.8	8	8	$\|\mathcal{D}\rangle$	98.5	
first exc.	4.0	10	10	$Q^{(1)+}\|gnd\rangle$	97* (87)	Fig. 6b (6a)
first exc.	2.0	10	10	$Q^{(1)+}\|gnd\rangle$	88 (60)	Fig. 7b (7a)
first exc.	2.0	10	8	$Q^{(1)+}\|gnd\rangle$	91* (71)	Fig. 10b (10a)
first exc.	1.2	10	10	$Q^{(1)+}\|gnd\rangle$	75 (46)	Fig. 8b (8a)
first exc.	1.2	10	8	$Q^{(1)+}\|gnd\rangle$	94 (84)	Fig. 11b (11a)

Table 2 (continued)

Exact State	G'	Projected Number, m	Average Number n	Quasi-boson State	Overlap (%)	Figure Reference
first exc.	1.2	10	8	$Q^{(1)+}S^{(0)+}\|gnd\rangle$	95*	Fig. 11c
first exc.	0.8	10	8	$Q^{(1)+}\|gnd\rangle$	99.3* (95)	Fig. 12b (12a)
first exc.	0.8	10	8	$Q^{(1)+}S^{(0)+}\|gnd\rangle$	97	Fig. 12c
first exc.	1.2	8	8	$Q^{(1)+}\|gnd\rangle$	97* (85)	Fig. 11b (11a)
first exc.	1.2	8	8	$Q^{(1)+}S^{(0)+}\|gnd\rangle$	95	Fig. 11c
first exc.	0.8	8	8	$Q^{(1)+}\|gnd\rangle$	98.9* (97.7)	Fig. 12b (12a)
first exc.	0.8	8	8	$Q^{(1)+}S^{(0)+}\|gnd\rangle$	98.8	Fig. 12c

Percentages above 99.95% are written 100%.

9. Conclusions

The main conclusion of Part II is that the numerical results in a simple model system show that the quasi-boson method can give useful approximations to the excitation energies and state vectors of at least the ground and first excited 0+ states of nuclear systems in the case of pairing potentials, provided that certain precautions are observed and certain revisions made in the method. The main precautions and revisions are:

(1) The zero energy boson used to help define the boson ground state should be

$$R^{(0)+} = Q^{(0)+} + f\, P^{(0)+}$$

and not simply $Q^{(0)+}$. (The bosons $R^{(0)+}$, $Q^{(0)+}$, $P^{(0)+}$, and the function f are defined in sections 4 and 5.) The use of $R^{(0)+}$ gives state vectors which are more concentrated in energy (less spread over exact excited states) and somewhat less concentrated in particle number.

(2) The first excited state for $G' \lesssim 1.2$ is a two boson state. For $\bar{\Delta} \neq 0$ (and this is the interesting case for reasons given in (3) below) the two bosons are one non-zero energy boson and one zero energy boson. (The arguments showing that this must be the case are developed in section 4.) The two boson nature of the first excited state may persist for G' at least as large as 1.2.

(3) The striking failure of the quasi-boson method for G' near 1 and average particle number, n, equal to a closed subshell, can be corrected by setting n slightly more or less than the closed subshell value. The resulting boson energies will be closer to the exact energies of the closed subshell system as a result of this slight displacement in n. The state vectors, though having their largest components at slightly incorrect particle number, are still useful, since a spread in particle number is characteristic of the approximation. The exact value of the change in n is not a critical parameter.

References to Part II

1) J. Högaasen-Feldman, Nuclear Physics 28 (1961) 258

2) A. M. Lane, Nuclear Theory (Benjamin, New York, 1964)

3) V. G. Soloviev, Atomic Energy Review, Vol. 3, No. 2 (International Atomic Energy Agency, Vienna, 1965) p. 117.

4) D. R. Bès, Nuclear Physics 49 (1963) 544

5) M. Rho and J. O. Rasmussen, Phys. Rev. 135 (1964) B1295
H. J. Mang, J. O. Rasmussen, and M. Rho, Phys. Rev. 141 (1966) 941

6) L. S. Kisslinger and R. A. Sorensen, Rev. Mod. Phys. 35 (1963) 853

7) A. Plastino, R. Arvieu, and S. A. Moszkowski, Phys. Rev. 145 (1966) 837.

PART III

EXACT DIAGONALIZATION IN SENIORITY TRUNCATED SPACES

1. Introduction

Parts I and II of this thesis are based on an approximate form for the grounds state vector of an even nuclear system. As noted in Part I, this form has one variational parameter per j-level of the nuclear system, instead of one coefficient for each possible configuration of the particles as in exact number conserving calculations. The use of the approximate state vector is thus based on the supposition, which is undoubtedly true for most deformed nuclear systems, that the dimensions of the matrices to be diagonalized in an exact number conserving calculation are impractically large for systems of more than a few particles outside of closed shells. (The dimensions of the matrices equal the numbers of configurations with given quantum numbers.) Also, the labor involved in claculating the many body matrix elements of the Hamiltonian may become prohibitive.

The development of computer technology, however, now allows matrices with dimension on the order of 200 or 300 to be diagonalized in one or two minutes of running time. Many calculations in spherical nuclear systems use matrices of less than this dimension.

The dimensions of matrices in exact calculations can be reduced by the method of seniority truncation[1]). The word seniority is used here in the following sense: a state created by n fermion particle creation operators

has seniority s of all but s of them are coupled pairwise to zero angular momentum. Thus a state of seniority zero must have total angular momentum zero. (The converse is not true. There are $J = 0$ states of seniority 4, 6, etc.) Seniority truncation is based on the observation that the dominant residual interaction in nuclei can be represented as an attractive potential which, in the j-j coupling scheme, acts most strongly in states of pairs of particles coupled to zero angular momentum. Therefore, configurations with more of these zero coupled pairs will generally lie lower in energy than those with fewer of them. Therefore, we will consider only the states of lowest seniority. When configurations are restricted to lowest seniority, it also becomes possible to obtain simple expressions for many body matrix elements of general two body operators.

2. Exact Diagonalization in Spaces of Seniority Zero and One

As before (eqs. (1) - (4) of Part I), we wish to find eigen vectors for a system of particles in shell model orbitals with single particle energy e_j, with configurations mixed by two body residual potential, V. As stated in Part I, the many body Hamiltonian operator is

$$H = \sum_j e_j n_j + \frac{1}{4} \sum_{\substack{i'j'ij \\ J}} \bar{G}(i'j'ijJ) \sum_M a^+_{i'j'}(JM)\, a_{ij}(JM) \tag{1}$$

with

$$n_j = \sum_m c^+_{jm}\, c_{jm} \tag{2}$$

$$a^+_{ij}(JM) = \sum_{qm} \langle iqjm|JM\rangle\, c^+_{iq}\, c^+_{jm} \;, \tag{3}$$

and

$$\bar{G}(i'j'ijJ) = \langle (i'j')JM|V|(ij)JM\rangle + (-1)^{i-j+J} \langle (i'j')JM|V|(ji)JM\rangle \tag{4}$$

Eq. (1) can also be written in the form conventional in pairing theory

$$H = \sum_j e_j n_j - \sum_{ij} G_{ij}\sqrt{\Omega_i}\sqrt{\Omega_j}\, a^+_i a_j + \frac{1}{4} \sum_{\substack{i'j'ij \\ J>0}} \bar{G}(i'j'ijJ)\, a^+_{i'j'}(JM)\, a_{ij}(JM) \tag{5}$$

where

$$G_{ij} = -\frac{\bar{G}(iijj0)}{[(2i+1)(2j+1)]^{1/2}} \tag{6}$$

and

$$a_j^+ = \frac{1}{\sqrt{2}}\, a_{jj}^+(00) \quad . \tag{7}$$

The states created by c_{jm}^+ are here specifically taken to be single particle levels in a certain harmonic oscillator potential well. The definition of the single particle wave functions, with a discussion of phases, is given in Appendix III-A. The phases are chosen such that the matrix elements above are real numbers.

Considering for the moment only a single level, labeled by j, the seniority zero (total J = 0) many particle state are denoted

$$|p\rangle = \mathfrak{n}_j^{-1}(p)\,(a_j^+)^p\,|0\rangle \tag{8}$$

where

$$0 \le p \le \Omega_j = \tfrac{1}{2}(2j+1) \quad ,$$

$$\mathfrak{n}_j^2(p) = \langle 0|(a_j)^p\,(a_j^+)^p|0\rangle \quad , \tag{9}$$

and where $|0\rangle$ is the state of no particles (vacuum state). The state $|p\rangle$ is thus a normalized state of p pairs in level j. The normalization factor, $\mathcal{N}_j(p)$, and certain other useful quantities, are derived in Appendix III-C for states of seniority zero, one and two.

Similarly, the states of seniority one (states of odd particle number) are

$$\overline{|p\rangle} = \bar{\mathcal{N}}_j^{-1}(p)\,(a_j^+)^p\, c_{jm}^+ |0\rangle \tag{10}$$

where

$$0 \leq p \leq \Omega_j - 1$$

and

$$\bar{\mathcal{N}}_j^2(p) = \langle 0|\, c_{jm}\,(a_j)^p\,(a_j^+)^p\, c_{jm}^+ |0\rangle \quad . \tag{11}$$

These are normalized states of 2p + 1 particles, p pairs plus one odd particle.

A convenient notation for configurations of particles in several j-levels is then, e.g., for seniority zero states,

$$|p\,q\,r\,s\cdots\rangle \tag{12}$$

where p is the number of pairs in the j-level with least e_j, q the number in the next least, etc. Thus, for a four

j-level treatment of the valance protons outside the Z = 28 closed shell in closed neutron shell nucleus ${}_{40}Zr^{90}_{50}$, some low lying configurations are

$$|3\ 2\ 1\ 0\rangle$$
$$|3\ 2\ 0\ 1\rangle$$
$$|3\ 1\ 1\ 1\rangle$$
$$\text{etc.}$$

where the configurations all have 6 pairs (12 protons) in the four levels. (The levels have j values 5/2, 3/2, 1/2, 9/2.) Similarly, some low lying configurations contained in the seniority one 5/2- state of ${}_{41}Nb^{91}_{50}$ are

$$|\bar{2}\ 2\ 1\ 1\rangle$$
$$|\bar{2}\ 2\ 0\ 2\rangle$$
$$|\bar{2}\ 1\ 1\ 2\rangle$$
$$\text{etc.}$$

The many body matrix elements of H in states such as eq. (12) are of the form,

$$\langle p'q'r'\cdots|H|pqr\cdots\rangle \qquad (13)$$

They can be calculated by the method of fractional parentage coefficients[1,2]) in which one begins with an unsymmetrized many particle state and then takes into account the complications introduced by anti-symmetrization. However, we have

defined our many particle states directly in terms of operators, c^{+}_{jm}, which have fermion anti-commutation relations. We therefore choose to evaluate expressions such as eq. (13) directly in terms of the commutation relations of the operators which define the potential and the states. These commutation relations are given in full generality in Appendix III-B. We note here only that

$$\left[a_{i'j'}(J'M'),\ a^{+}_{ij}(JM) \right] \tag{14}$$

has a constant term plus terms containing operators of the form

$$n_{ij}(K\mu) = -\sum_{qm} \langle i q j m | K\mu \rangle\, c^{+}_{iq}\, (-1)^{j-m}\, c_{j\,-m} \tag{15}$$

for all

$$|J-J'| \leq K \leq J+J'$$

and

$$\mu = M - M'$$

When K and μ are zero, eq. (15) becomes

$$n_{ij}(00) = \frac{\delta_{ij}}{\sqrt{(2j+1)}} \sum_m c^+_{jm} c_{jm} = \frac{\delta_{ij}}{\sqrt{(2j+1)}} n_j$$

where n_j is defined in eq. (2). The commutation relation

$$[n_{i'j'}(J'M'), a^+_{ij}(JM)] \tag{16}$$

consists of terms with operators of the form

$$a^+_{ij}(K\mu)$$

with $K\mu$ given in terms of the J, M, J', M', just as above in eq. (15).

All of the many body matrix elements relevant to a general potential acting in seniority zero and one states are derived and listed in Appendix III-D. A few of them are listed here to show their simplicity.

$$\langle p | a^+_j a_j | p \rangle = \frac{p(\Omega_j - p + 1)}{\Omega_j}$$

$$\langle p | a^+_{jj}(JM)\, a_{jj}(JM) | p \rangle = \frac{2p(p-1)}{\Omega_j(\Omega_j - 1)} \tag{17}$$

$$\langle q\, p | a^+_{ij}(JM)\, a_{ij}(JM) | q\, p \rangle = \frac{q}{\Omega_i} \frac{p}{\Omega_j}$$

Only the pairing term, the term with coefficient G_{ij} in eq. (5), is effective in mixing configurations.

The matrix elements of the $J > 0$ terms are independent of the J, M quantum numbers. Therefore, defining

$$G^{(2)}_{ij} = \sum_{J>0} (2J+1)\, \bar{G}(ij\,ij\,J) \tag{18}$$

we may write H in a form which is equivalent to eq. (5) in seniority zero and one states,

$$H = \sum_j e_j n_j - \sum_{ij} G_{ij}\sqrt{\Omega_i}\sqrt{\Omega_j}\, a_i^{+} a_j + \frac{1}{4}\sum_{ij} G^{(2)}_{ij}\, a^{+}_{ij}(J0)\, a_{ij}(J0) \tag{19}$$

where the last term is evaluated for each i, j by setting nonzero J to any value for which the operator $a^{+}_{ij}(J0)$ is nonzero.

A computer program which calculates and diagonalizes the matrix of H in seniority zero and one systems is listed in Appendix III-E.

3. Quasi-spin

The matrix elements of general forces in seniority zero and one many particle states have been derived using the commutation relations of certain operators. We might wonder if the Hamiltonian, eqs. (5) or (19), can be written in terms of some set of operators which is closed under the operation of commutation. The difficulty is that the terms, eq. (15), that result from the commutation of a^+ and a have all values of angular momentum K from $|J - J'|$ to $(J + J')$. Then the commutation of each of the n operators, eq. (16), yields still more K values, and so on until all possible J values have been reached.

For a pure pairing force, however, there is only one value, J = 0. We then have the simple commutation relations

$$[a_i , a_j^+] = \delta_{ij} \left(1 - \frac{n_j}{\Omega_j}\right)$$

$$[n_i , a_j^+] = 2\delta_{ij} a_j^+$$

which show that the set of operators a_j^+, a_j, n_j is indeed closed under commutation. In fact, it has been noted[3]) that the operators $S_j^{(+)}$, $S_j^{(-)}$, and $S_j^{(z)}$ defined by

$$S_j^{(+)} = \sqrt{\Omega_j}\, a_j^+$$

$$S_j^{(-)} = \sqrt{\Omega_j}\, a_j$$

$$S_j^{(z)} = \frac{1}{2}\left(n_j - \Omega_j\right) \tag{20}$$

obey the same commutation relations as the angular momentum operators J_+, J_-, J_z. The pure pairing Hamiltonian can be written in terms of the S_j operators

$$H = \sum_j e_j\left(2S_j^{(z)} + \Omega_j\right) - \sum_{ij} G_{ij}\, S_i^{(+)} S_j^{(-)} \tag{21}$$

The states we have labeled by $|p\rangle$ are then labeled $|\tilde{j}\,\tilde{m}\rangle$ where $\tilde{j}$ $\tilde{m}$ are quasi-spin quantum numbers

$$\tilde{j} = \frac{1}{2}\Omega_j$$

$$\tilde{m} = \frac{1}{2}\left(2p - \Omega_j\right)$$

If $G_{ij} = G$ (constant pairing potential), and also $e_j = e$ for all j,

$$H = e\left(2S^{(z)} + \Omega\right) - G\, S^{(+)} S^{(-)} \tag{22}$$

where

$$S^{(+)} = \sum_j S_j^{(+)}$$

$$S^{(-)} = \sum_j S_j^{(-)}$$

$$S^{(z)} = \sum_j S_j^{(z)}$$

have the same commutation relations as those of the S_j operators in eq. (20).

If all the e_j are equal, the quasi-spin formalism can give eigen vectors of H by the method of vector coupling of the quasi-spins of the individual j-levels. However, this result is not true when the e_j are unequal; the formalism is then a somewhat inconvenient method of calculating the many body matrix elements, eq. (13). For this reason, we do not use it for that purpose in this paper.

4. The Delta-function Potential

The delta-function two body residual potential,

$$V(\bar{r}_1, \bar{r}_2) = -V_\delta \, \delta(\bar{r}_1 - r_2) \tag{23}$$

unlike the pure pairing potential, has a somewhat realistic spatial significance. It represents the limit of a short range attractive potential of great depth. Nonetheless, it has algebraic properties which are as simple as, or simpler than[4]), those of the pure pairing potential. The well known derivation[1]) of the identical particle two body diagonal matrix elements of eq. (23) has been generalized[5]) to give

$$G(i'j'ijJ) = 0$$

when $(l_i + l_j + J)$ is odd, and

$$\bar{G}(i'j'ijJ) = -V_\delta (-1)^{i'-i+\frac{1}{2}(\ell_{i'}-\ell_i+\ell_j-\ell_{j'})} \times$$

$$\times \frac{(\hat{i}'\hat{j}'\hat{i}\hat{j})^{\frac{1}{2}}}{\hat{J}} \langle i'\tfrac{1}{2}\, j'-\tfrac{1}{2} | J0\rangle \langle i\tfrac{1}{2}\, j-\tfrac{1}{2} | J0\rangle \, I_{i'j'ij} \tag{24}$$

when $(l_i + l_j + J)$ is even, where

$$\hat{j} = (2j+1)$$

and

$$I_{i'j'ij} = \frac{1}{4\pi}\int_0^\infty \frac{dr}{r^2} R_{i'}(r)\, R_{j'}(r)\, R_i(r)\, R_j(r) \quad . \tag{25}$$

The radial wave functions and the integral, eq. (25), are treated in detail in Appendix III-A. A program to compute the integrals is listed in Appendix III-E.

Let the delta-potential, eq. (23), act in seniority zero and one states. It follows that the parameters defined in eqs. (6) and (18) are

$$G_{ij} = V_\delta\, I_{iijj} \tag{26}$$

$$G^{(2)}_{ij} = -V_\delta (2i+1)(2j+1)\, I_{ijij} \sum_{\substack{J>0 \\ \ell_i+\ell_j+J \\ \text{even}}} \langle i\tfrac{1}{2}\, j\, -\tfrac{1}{2} | J0 \rangle^2 \tag{27}$$

The following identity[4]),

$$\sum_{\substack{J \\ \ell_i+\ell_j+J \\ \text{even}}} \langle i\tfrac{1}{2}\, j\, -\tfrac{1}{2} | J0 \rangle^2 = \frac{1}{2} \tag{28}$$

gives immediately

$$G^{(2)}_{ij} = -V_\delta (2i+1)(2j+1)\, I_{ijij} \left(\frac{1}{2} - \frac{\delta_{ij}}{2j+1}\right) \tag{29}$$

or

$$G_{ij}^{(2)} = -2\Omega_i(\Omega_j - \delta_{ij})G_{ij} \tag{30}$$

since $I_{ijij} = I_{iijj}$ from the definition, eq. (25).

If we set all radial integrals I_{iijj} equal, we obtain what is called surface delta interaction. This name refers to arguments that if the attractive short range potential were mostly effective in the nuclear surface region, the effect would be a smoothing out of variations in the radial integrals. Setting

$$V_\delta I_{iijj} = G \tag{31}$$

we obtain $G_{ij} = G$ in eq. (26). We see from eq. (5) that the $J = 0$ term of a surface delta potential is a constant pairing potential. The relation, eq. (30), remains valid, of course. It has been demonstrated[4]) that the surface delta interaction can be expressed as the sum of a quasi-spin scalar and a term which depends only on the total number of particles. For reasons given at the end of section 3, we do not use this result in calculations. However, the surface delta interaction itself will be used in the following sections since it has only the one free parameter, G, and yet has spatial significance as a short range attractive potential.

5. Nickel Isotopes

The method of exact diagonalization in seniority zero and one spaces is here used to calculate the ground and excited 0+ states of even isotopes of nickel and the low lying half integral angular momentum states of odd isotopes of nickel. The nickel isotopes are treated as a system of valence neutrons outside of the closed neutron shell at N = 28. (The protons, with Z = 28, also form a closed shell, and are also assumed not to be excited.)

Previous theoretical studies of the isotopes of nickel, e.g. refs.[6,7,8]), have generally taken the single particle energies of the j-levels, e_j, from the experimental excitation energies of ${}_{28}Ni^{57}_{29}$, which has one neutron outside the 28-28 doubly closed shell. In ref.[8]), a least squares method is used to determine the two body residual potential which best fits the energies of the low lying excitation spectra and the binding energies of Ni isotopes from Ni^{58} to Ni^{65}. In such a calculation, any changes in the single particle neutron energies, e_j, as N varies from 29 to 37 (Ni^{57} to Ni^{65}) are assumed to be included in the effective residual potential. The best fit potential from ref.[8]) turns out to have repulsive $G^{(2)}_{ij}$ parameters. In fact, the parameters G_{ij} and $G^{(2)}_{ij}$ (defined in eqs. (6) and (18) above) of the potential of ref.[8]) are similar to those of a pure, constant pairing potential with G = 0.9 MeV, added to a repulsive surface delta

potential of strength G = -0.5 MeV. (In our convention G > 0 for attractive potentials.)

The study[6]), on the other hand, used an attractive surface delta interaction and obtained qualitative agreement with the spectra of several Ni isotopes (including agreement with the first 2+ excitation energies in some even Ni isotopes). The qualitative success of this study[6]) seems to raise the possibility that, if changes in the e_j from isotope to isotope are explicitly included in the calculation, a reasonable fit to the Ni data might be obtained with a simpler potential than that of ref.[8]).

The present study uses an attractive surface delta force. It assumes that the 28-28 core is inert in the sense that nucleons are not excited from it into valence states. But it assumes that the core-valence binding, the e_j, may vary with neutron number, N. We may say that the core is inert but variable. In order for the binding energies of the various ground states to have a simple significance, we assume also that the core-core contribution to the binding energy does not vary with neutron number, N. Then the quantity (see eqs. (6), (7) of ref.[8])

$$B(n) = -\left\{ B.E.(Ni^{56+n}) - B.E.(Ni^{56}) - 10.26n \right\} \tag{32}$$

corresponds to the lowest eigen value of H in each isotope (model absolute ground state energy). For convenience,

we have chosen the zero of energy at the ground state of Ni^{57} which is bound by 10.26 MeV relative to Ni^{56}. If the assumption of constant core-core binding is invalid, the result is that effects of changes in core-core binding energy are included in the e_j parameters, and in the potential V.

The present study attempts to fit the seniority zero and one spectra, and the ground state binding energies, B(n), of the isotopes of Ni. But in order to avoid a proliferation of adjustable parameters, we seek a fit with a smooth variation in the e_j values as neutron number increases, preferably a variation that can be parameterized economically. The diagonalization is performed in a system of three single particle neutron valence states, $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$.

We first tested the effects of seniority truncation by using the two body matrix elements of ref.[8]) to calculate the seniority zero and one energies. The energies obtained fit well with those obtained by the non-seniority-truncated treatment of ref.[8]). (The rms theory-theory difference is 80 KeV for 20 states.) Since the surface delta potential conserves seniority in single j-levels[1]) and conserves quasi-spin in systems of many j-levels[4, 18]), we expect seniority truncation to be an even better approximation for a surface delta potential than it is for the potential of ref.[8]). Therefore, the effects of seniority truncation of the energy spectra in the present study are probably less than the above 80 KeV figure.

The results of the study are shown in table 1. The e_j levels are parameterized linearly,

$$e_j^{(A)} = \alpha_j + \beta_j (A - 57) \tag{33}$$

which requires two parameters for each of the three j-levels. These five parameters ($\alpha_{3/2} = 0$ by assumption), plus the potential strength G, make six parameters to adjust in fitting 23 experimental energies. The numbers in parentheses are the values of B(n) for the ground states. The experimental energies for each isotope are in the row immediately following the calculated values. The fit obtained is somewhat crude. The 14 excitation energies have a 211 KeV rms difference from the experimental values. This compares to an rms difference of 227 KeV obtained in ref.[8]). Of course, the least squares fit of ref.[8]) included many more states than the present work. The binding energies are not fit well. They have a 454 KeV rms difference with the experimental (based on the assumption of constant core) B(n) values. The errors in the even-A binding are systematically greater than those in the odd-A, which suggests that a stronger potential would improve the fit to the binding energies. The value G = 0.45 MeV was chosen to give about the right 0+ excitation energies in the even-A nuclei. It is probable that a systematic least squares fit, varying the α_j , β_j , and G would give better agreement with experiment.

Table I

A	$e_{3/2}$ ($\beta_{3/2}$ = 0.24)	$e_{5/2}$ ($\beta_{5/2}$ = 0.17)	$e_{1/2}$ ($\beta_{1/2}$ = 0.14)	E_{0+}	E^*_{0+}	$E_{3/2}$	$E_{5/2}$	$E_{1/2}$
57	$\alpha_{3/2}=0$	$\alpha_{5/2}=0.78$	$\alpha_{1/2}=1.08$	-	-	(0)	0.78	1.08
				-	-	(0)	0.78^e	1.08^e
58	0.24	0.95	1.22	(-1.38)	2.64	-	-	-
				$(-1.93)^e$	2.77^e	-	-	-
59	0.48	1.12	1.36	-	-	(-0.37)	0.33	0.52
				-	-	$(-0.67)^e$	0.34^e	0.47^e
60	0.72	1.29	1.50	(-1.16)	2.43	-	-	-
				$(-1.80)^e$	2.29^e	-	-	-
61	0.96	1.46	1.64	-	-	(0.90)	0.03	0.11
				-	-	$(0.64)^e$	0.07^e	0.28^e
62	1.20	1.63	1.78	(0.73)	2.69	-	-	-
				$(0.31)^e$	2.05^e	-	-	-
63	1.44	1.80	1.92	-	-	0.10	0.00	(3.76)
				-	-	0.16^e	0.09^e	$(3.73)^e$

Table I (cont'd.)

A	$e_{3/2}$	$e_{5/2}$	$e_{1/2}$	E_{0+}	E^*_{0+}	$E_{3/2}$	$E_{5/2}$	$E_{1/2}$
64	1.68	1.97	2.06	(4.18)	2.58	-	-	-
				$(4.33)^e$	2.89^e	-	-	-
65	1.92	2.14	2.20	-	-	0.14	(7.78)	-0.01
				-	-	0.32^e	$(8.46)^e$	0.06^e
66	2.16	2.31	2.34	(9.19)	2.62	-	-	-
				$(9.76)^e$		-	-	-

G = 0.45 MeV

Rms differences between calculation and experiment:

211KeV for 14 excitation energies

454KeV for 9 binding energies

Experimental quantities (taken from ref. [8]) are marked with superscript e.

All energies in table above are in MeV.

The study demonstrates that reasonable agreement with the low lying spectra of the Ni isotopes can be obtained using seniority truncation and a surface delta potential. The study also illustrates the utility of the method of exact diagonalization in the study of features of nuclear spectra. A particular advantage of the method used here is that the number of single particle levels can be increased from three to include also the $1f_{7/2}$ and $1g_{9/2}$ levels. This addition of j-levels does not appreciably increase the complexity of the calculation.

6. Fifty Neutron Nuclei

The method of exact diagonalization in seniority zero and one states is applied to nuclei with a closed, N = 50, neutron shell and with valence protons outside of the closed shell at Z = 28. The experimental spectra of the 50 neutron nuclei are not so well known as those of the Ni isotopes. Therefore, no fitting of energy levels using variable e_j values will be attempted here. Instead, the single particle energies will be chosen to fit reasonably the levels of ${}_{39}Y^{89}_{50}$ and ${}_{41}Nb^{91}_{50}$. These levels will then also be used in the diagonalization of ${}_{38}Sr^{88}_{50}$ and ${}_{40}Zr^{90}_{50}$.

The single particle proton valence levels are $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, and $1g_{9/2}$. These are all of the single particle levels between the Z = 28 and Z = 50 shell closures. The single particle proton energies used

$$e_{5/2} = 0.00 \text{ MeV}$$
$$e_{3/2} = 0.25$$
$$e_{1/2} = 1.80$$
$$e_{9/2} = 2.90$$

are similar to those used in other calculations in these nuclei (e.g., see ref.[9]). The diagonalizations are performed with both a pure, constant pairing potential, and a surface delta potential. The potential strength, G, is taken to be the usual[9]) value determined by quasi-particle methods from the odd-even mass difference. In this case, it is $G \approx 22/A$ MeV

(= 0.25 MeV when A = 90). The calculated excitation energies are compared with known experimental values in table 2, for five of the 50 neutron nuclei, Sr, Y, Zr, Nb, Mo.

The (number conserving) state vectors from the above diagonalization are used to calculate the ρ^2 values of the excited 0+ to ground 0+ electric monopole transitions in Zr, Sr, and Mo. The quantity ρ^2 is defined by

$$\rho^2 = \left| \langle \text{exc. } 0+ | \sum_i \left\{ \left(\frac{r_i}{R}\right)^2 - \sigma \left(\frac{r_i}{R}\right)^4 + \cdots \right\} | \text{gnd } 0+ \rangle \right|^2 \qquad (34)$$

where the sum, i, runs over all protons and where

$$R = 1.2 \times 10^{-13} \, A^{\frac{1}{3}} \text{ cm}.$$

(The parameter A is the atomic number of the nucleus.) The ρ^2 value is a conventional measure, similar to the B(E2) value for electric quadrupole transitions, of the nuclear part of the expression for the rate of electric monopole transitions. These transitions proceed mainly by the excitation of K-shell electrons. The parameter, σ, above, is determined from an assumed nuclear charge distribution. (See fig. 5 of ref.[10].) For nuclei in the region of Zr, an average value of σ is $\sigma = 0.025$.

In a harmonic oscillator single particle basis, such as the one which we are using, the one body operator, r^2, between

Table 2

Nucleus	E_{0+}	E^*_{0+}	ρ^2	$E_{5/2-}$	$E_{3/2-}$	$E_{1/2-}$	$E_{9/2+}$
$_{38}Sr^{88}$	0	2.41	0.002	-	-	-	-
				-	-	-	-
$_{39}Y^{89}$	-	-	-	1.54	1.30	0	1.00
	-	-	-	1.74^e	1.51^e	0^e	0.91^e
$_{40}Zr^{90}$	0	1.76	0.023	-	-	-	-
	0	1.75^e	0.0031^e	-	-	[illegible]	-
$_{41}Nb^{91}$	-	-	-	1.69	1.45	0.12	0
	-	-	-			0.11^e	0^e
$_{42}Mo^{92}$	0	2.41	0.017	-	-	-	-
				-	-	-	-

Experimental energies (taken from ref.[14]) and the experimental ρ^2 value (taken from ref.[15]) are marked with superscript e.
All energies are in MeV.

orthogonal states (the ground and excited 0+ states in eq. (34) are orthogonal) is proportional to an operator which counts the number of particles in the j-levels with oscillator radial quantum number one more or less than the oscillator radial quantum number of the majority of j-levels in the calculation. (In many calculations, there is only one j-level of different oscillator radial quantum number.) In the present calculation, the $g_{9/2}$ level has radial quantum number 4, and the other three levels have radial quantum number 3. The ρ^2 thus is sensitive to the occupancy of the $g_{9/2}$ level, and to the relative ground and excited state signs of the coefficients of configurations with the $g_{9/2}$ level occupied. A program to compute ρ^2 using matrix elements of r^2 and r^4 from ref.[11]) is listed in Appendix III-D.

There is a wide disagreement (see table 2) between the one experimentally measured ρ^2 value and the calculated value, in Zr^{90}. The calculated value is seven times too large. Fig. 1 shows the values of ρ^2 and 0+ excitation energies for a range of G values in Zr^{90}, using a constant, pure pairing potential. It is seen that agreement between the calculated and experimental values of both quantities is obtainedfor a low pairing potential strength, G = 12.5/90 MeV. The excitation energies in Nb and Y also agree will with experiment at this G value.

The low value of G, G = 12.5/90 MeV, seems to be ruled

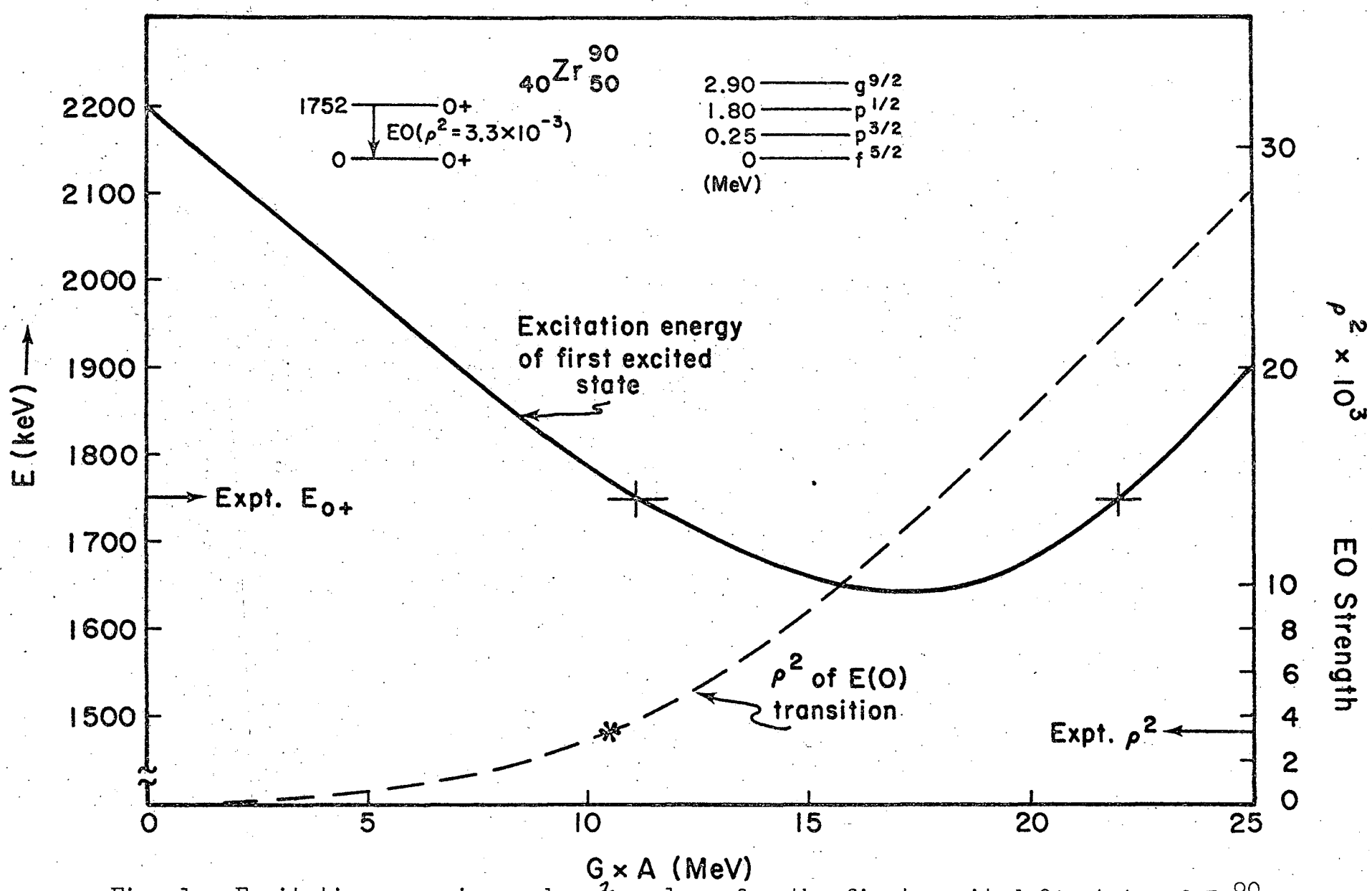

Fig. 1. Excitation energies and ρ^2 values for the first excited 0+ state of Zr^{90}, shown for various values of potential strength, G.

out, however, by consideration of the odd-even binding energy differences in 50 neutron nuclei. (The low value also gives poor agreement with nucleon transfer data shown in table 4.) The strong attractive pairing component in residual nuclear forces leads to a systematically greater binding energy in even-even nuclei (N, Z both even, e.g. Zr^{90}, Sr^{88},...) than in even-odd nuclei (here, N even, Z odd, e.g. Nb^{91}, Y^{89}, ...). This odd-even difference adds a discontinuous part to the smooth dependence of binding energy on Z. Thus the binding energy of N = 50 nuclei may be represented

$$B(Z) = g(Z) + \delta(Z) \tag{36}$$

where g(Z) is a smooth function and

$$\begin{aligned} \delta(Z) &= 0 && \text{Z odd} \\ &= \delta && \text{Z even} \end{aligned} \tag{37}$$

We wish to correlate the magnitude of δ with the magnitude of the pairing potential in N = 50 nuclei. To do this, we note that, while the second derivative of g(Z) with respect to Z for fixed N is large, the third and higher derivatives are small compared to the magnitude of δ. (The second derivative of the semi-empirical mass formula for fixed N is about -900 KeV at Zr^{90}.) We therefore form a three point approximation to the second derivative

$$P_2(z) = \frac{1}{2}\left\{ B(z+1) + B(z-1) - 2B(z) \right\} . \tag{38}$$

From eqs. (36) and (37)

$$P_2(z) \approx \frac{1}{2} \frac{\partial^2 g}{\partial z^2} \pm \delta \tag{39}$$

with the plus sign when Z is odd. Since $\partial^2 g / \partial z^2$ is large, we form the four point approximation[17]) to the 3rd derivative

$$P_3\left(z + \tfrac{1}{2}\right) = P_2(z+1) - P_2(z) \tag{40}$$

which is, approximately,

$$P_3\left(z + \tfrac{1}{2}\right) \approx \frac{1}{2} \frac{\partial^3 g}{\partial z^3} \pm 2\delta \tag{41}$$

Since $\partial^3 g / \partial z^3$ is small, we are left with the term in δ . To be safe, we can also compute

$$P_4(z) = \frac{1}{2}\left\{ P_2(z+1) + P_2(z-1) - 2P_2(z) \right\} \tag{42}$$

which is, approximately,

$$P_4(z) \approx \frac{1}{4} \frac{\partial^4 g}{\partial z^4} \pm 2\delta . \tag{43}$$

The terms in δ, being discontinuous, persist through this series of differences.

Table 3 shows the above quantities computed for the 50 neutron nuclei. The experimental binding energies are from ref.[11]). Note that the P_3 and P_4 columns are of about the same magnitude. This indicates that the continuous part of the binding energy (g(Z) above) is already negligible in P_3. Table 3 shows the same quantities calculated for minus the ground state absolute eigen energies, taken from the exact diagonalization of a surface delta potential with G = 0.25 MeV. (These numbers differ from binding energies by a linear term which does not affect P_2.) The calculated quantities, table 3a, are about 2/3 of the experimental ones, table 3. This indicates that the pairing potential should be increased somewhat to obtain agreement. A decrease of G from 22/90 to 12.5/90 MeV to obtain agreement with ρ^2 would, therefore, lead to strong disagreement with the experimental odd-even binding energy difference. It is interesting that in both table 3 and table 3a, the closure of the $p_{1/2}$ subshell at Zr^{90} leads to an increase in δ as the $g_{9/2}$ level is filled. This effect, due to the increased $g_{9/2}$ pairing self-energy, is supporting evidence for the correctness of the model being used.

The incorrect prediction for ρ^2 above can perhaps be explained by saying that all electric transition rate calculations are subject to errors introduced by what are

Table 3

N = 50 Nuclei	B.E.	$P_2(Z)$	$P_3(Z)$	$P_4(Z)$
$_{35}Br^{85}$	737 440			
$_{36}Kr^{86}$	749 213	-1573		
$_{37}Rb^{87}$	757 840	992	2565	-2566
$_{38}Sr^{88}$	768 450	-1575	-2567	2286
$_{39}Y^{89}$	775 910	430	2005	-2090
$_{40}Zr^{90}$	784 230	-1745	-2175	2730
$_{41}Nb^{91}$	789 060	1540	3285	-3413
$_{42}Mo^{92}$	796 970	-2000	-3540	
$_{43}Tc^{93}$	800 880			

All energies are in KeV.

Experimental binding energies are taken from ref.[12]).

Table 3a

N = 50 Nuclei	$-E_0$	$P_2(Z)$	$P_3(Z)$	$P_4(Z)$
$_{35}Br^{85}$	3755			
$_{36}Kr^{86}$	5098	-833		
$_{37}Rb^{87}$	4736	784	1617	
$_{38}Sr^{88}$	5941	-1003	-1787	-1701
$_{39}Y^{89}$	5141	465	1468	1628
$_{40}Zr^{90}$	5271	-893	-1358	-1413
$_{41}Nb^{91}$	3615	947	1840	1599
$_{42}Mo^{92}$	3852	-972	-1919	-1880
$_{43}Tc^{93}$	2145			

All energies are in KeV.

called effective charge effects. The assumptions of inertness for the neutron system and the Z = 28 proton core may be too stringent to allow correct prediction of ρ^2. This is particularly likely since the ρ^2 value is seen to depend on small components of the state vectors. It is also possible that the assumption of harmonic oscillator single particle wave functions is incorrect. The form of the r^2 matrix element may, therefore, properly include terms other than the ones used in the calculation above.

Another kind of experimental quantity which we can calculate using the exact, number conserving state vectors, is spectroscopic factors of one proton stripping and pick-up reactions. These spectroscopic factors, the nuclear state vector parts of the stripping and pick-up cross sections, are defined

$$\mathcal{S}_j(a \rightleftarrows b) = \frac{1}{2j_b+1} \left| \frac{\langle j_b m_b | c^{+}_{jm} | j_a m_a \rangle}{\langle j m \, j_a m_a | j_b m_b \rangle} \right|^2 \qquad (44)$$

where the forward arrow refers to stripping (adding one particle to the nucleus) and the backward arrow to pick-up (taking one particle out of the nucleus). Note that the names were coined by particle physicists, not by nuclear structure physicists.

Recent experimental measurements[13]) have been performed for the pick-up reactions

$$Zr^{90}(d, He^3)Y^{89},$$

$$Y^{89}(d, He^3)\, Sr^{88}$$

which have spectroscopic factors, for Zr and Sr in 0+ states,

$$\mathcal{S}_j^{(Zr)} = (2j+1)\left| \langle Y^{89}_{(j)} \,|\, c_{j-m} \,|\, Zr^{90} \rangle \right|^2$$

and (45)

$$\mathcal{S}_{1/2}^{(Sr)} = 2\left| \langle Y^{89}_{(1/2)} \,|\, c^{+}_{1/2\, m} \,|\, Sr^{88} \rangle \right|^2$$

respectively. The factors in eq. (45) have the following sum rule

$$\frac{1}{2j+1} \sum_k \mathcal{S}_j^{(Zr)}(k) = \frac{\langle Zr^{90} | n_j | Zr^{90} \rangle}{2j+1} \qquad (46)$$

where the number on the right hand side of eq. (46) is the fractional occupation number of the level j in the Zr^{90} ground state. The sum k is over all states of Y^{89} with the same quantum numbers as the lowest state of given j. The spectroscopic factors obtained by calculation, using constant, pure pairing potential of magnitudes G = 12.5/90 and G = 21.5/90 MeV are shown in table 4, along with experimental values from ref.[13]). The calculations are done using a computer program (Appendix III-E) based on the easily derivable expressions

Table 4

$Zr^{90}_{(0)}$ (d, He^3) $Y^{89}_{(j)}$

j	G = 12.5/90 MeV	G= 21.5/90 MeV	Expt. (ref[13])
1/2-	0.950	0.775	0.57
1/2-*	0.000	0.005	
9/2+	0.012	0.065	0.051
9/2+*	0.004	0.011	
3/2-	0.993	0.962	0.55
3/2-*	0.000	0.002	
5/2-	0.994	0.969	0.33
5/2-*	0.000	0.001	

$Y^{89}_{(1/2-)}$ (d, He^3) $Sr^{88}_{(J)}$

J	G = 12.5/90 MeV	G = 21.5/90 MeV	Expt. (ref.[13])
0+	0.983	0.915	1.000†
0+*	0.016	0.079	0.000

† Defined as unity in ref.[13]) to normalize data.

Entries are reduced spectroscopic factors $S_j/(2j+1)$.

$$\langle \overline{p} | c^{+}_{jm} | p \rangle = \left(\frac{\Omega_j - p}{\Omega_j} \right)^{\frac{1}{2}}$$

$$\langle \overline{p-1} | c_{j-m} | p \rangle = \left(\frac{p}{\Omega_j} \right)^{\frac{1}{2}} \qquad (47)$$

The authors of the paper[13]) suggest that the experimental numbers are reliable to about 20% of their magnitudes, except for the pick-up factor to the 5/2- level of Y^{89}, which they consider less reliable. The experimental factor for the Sr^{88} ground state is defined by the authors[13]) to be 1.00. They assume no configuration mixing in Sr^{88}. While our calculation disagrees with this assumption, we do not renormalize the other spectroscopic factors because of the fairly large error inherent in them anyway. We note from table 4 that the calculation with G = 21.5/90 MeV is in fairly good agreement with experiment for the 1/2- and 9/2+ levels in Y^{89}, while the calculation with G = 12.5/90 MeV is not in agreement. The disagreement between calculated and experimental pick-up factors to the 3/2- level in Y^{89} may indicate that a much stronger potential is needed to reduce the occupancy of the states of lower e_j in Zr^{90}.

In summary, then, the calculations of N = 50 nuclei using pairing and surface delta potentials of strength $G \approx 22/90 = 0.25$ MeV give satisfactory agreement with

experimental excitation energies, odd-even binding energy differences, and spectroscopic factors of pick-up reactions from Zr^{90} to the lowest excited states of Y^{89}. The agreement with the ρ^2 value of the E0 transition in Zr^{90} is unsatisfactory, but may be due to the effect of core excitations not included in the calculations.

7. Eighty-two Neutron Nuclei

A study similar to that of section 6 preceeding has also been made for nuclei with a closed neutron shell at N = 82 neutrons. The seniority zero and one states of valence protons outside of the Z = 50 closed proton shell are treated, using a surface delta potential. The single particle valence proton states used are $1g_{7/2}$, $2d_{5/2}$, $1h_{11/2}$ with energies similar to those of ref.[9]),

$$e_{7/2} = 0.00 \text{ MeV}$$
$$e_{5/2} = 0.60$$
$$e_{11/2} = 2.00$$

The surface delta potential strength is taken to be G = 0.18 MeV. The tables 5 and 5a show the same quantities, P_2, P_3, P_4, as in section 6, eqs. (38) - (43), for the experimental and calculated binding energies respectively. Comparison of the two tables shows that the choice of G = 0.18 MeV gives approximate agreement with experimental odd-even binding energy differences.

The calculated excitation energies of nuclei from Z = 54 to Z = 62 are shown and compared with experimental values in table 6. Reasonable agreement with the few measured values is obtained. Note that the calculation predicts the existence of two closely spaced excited 0+ states in Sm.

Table 5

N = 82 Nuclei	B(Z)	$P_2(Z)$	$P_3(Z)$	$P_4(Z)$
$_{54}Xe^{136}$	1 141 854			
$_{55}Cs^{137}$	1 149 520	652		
$_{56}Ba^{138}$	1 158 490	-1325	-1977	2071
$_{57}La^{139}$	1 164 810	840	2165	-2170
$_{58}Ce^{140}$	1 172 810	-1335	-2175	2225
$_{59}Pr^{141}$	1 178 140	940	2275	-2363
$_{60}Nd^{142}$	1 185 350	-1510	-2450	2558
$_{61}Pm^{143}$	1 189 540	1155	2665	
$_{62}Sm^{144}$	1 196 040			

All energies are in KeV.

Experimental binding energies are taken from ref.[12]).

Table 5a

N = 82 Nuclei	$-E_0$	$P_2(Z)$	$P_3(Z)$	$P_4(Z)$
$_{54}Xe^{136}$	3012			
$_{55}Cs^{137}$	2817	879		
$_{56}Ba^{138}$	4379	-955	-1834	1879
$_{57}La^{139}$	4031	970	1925	-1958
$_{58}Ce^{140}$	5623	-1022	-1992	2005
$_{59}Pr^{141}$	5172	997	2018	-2012
$_{60}Nd^{142}$	6714	-1028	-2025	2012
$_{61}Pm^{143}$	6200	972	2000	
$_{62}Sm^{144}$	7629			

All energies are in KeV.

Table 6

Nucleus	E_{0+}	E^*_{0+}	ρ^2	$E_{7/2+}$	$E_{5/2+}$	$E_{11/2-}$
$_{54}Xe^{136}$	0	2.18	9.3×10^{-5}	-	-	-
				-	-	-
$_{55}Cs^{137}$	-	-	-	0	0.30	1.54
	-	-	-			
$_{56}Ba^{138}$	0	2.01	1.7×10^{-4}	-	-	-
				-	-	-
$_{57}La^{139}$	-	-	-	0	0.09	1.24
	-	-	-	0^e	0.17^e	
$_{58}Ce^{140}$	0	1.89	2.7×10^{-4}	-	-	-
	0	1.90^e	0.017^e	-	-	-
$_{59}Pr^{141}$	-	-	-	0.11	0	0.98
	-	-	-	0.15^e	0^e	
$_{60}Nd^{142}$	0	2.12	3.8×10^{-4}	-	-	-
	0	2.21^e		-	-	-
$_{61}Pm^{143}$	-	-	-	0.30	0	0.77
	-	-	-			
$_{62}Sm^{144}$	0	2.46, 2.51	4.9×10^{-4}	-	-	-
	0	1.67^e, 2.44^e		-	-	-

Experimental energy values (taken from ref.[14]), and the experimental ρ^2 value (taken from ref.[16]), are marked with superscript e.

The ρ^2 parameter discussed in section 6, eq. (34), is also calculated for even nuclei. The agreement with the one measured value, in Ce^{140}, is poor. The small value calculated is due to an incoherence in signs of the state vector coefficients between the ground 0+ and excited 0+ states, which leads to cancellation of the larger contributions to ρ^2. Here, even more than in the case of Zr^{90} in section 6, we would expect core excitations to play a significant role. Also, as in section 6, the assumption of harmonic oscillator single particle wave functions may be overly restrictive.

The calculation gives good qualitative agreement with the measured excitation energies and binding energy differences.

8. Conclusion

In Part III of this thesis, we have developed a method of exact number conserving diagonalizations of the many body Hamiltonian matrix, in seniority truncated configuration spaces. This method has been developed in a form which can be used with general two body residual forces.

The method of exact diagonalization has been illustrated by studies of the Ni isotopes, 50 neutron isotopes, and 82 neutron isotopes. The Ni study, in particular, illustrates that the exact method can be used to investigate alternative interpretations of the shell model, without the uncertain effects of quasi-particle approximations on the results obtained. The method of exact diagonalizations outlined here is conceptually simple and yet no more complicated computationally than alternate, quasi-particle methods.

References to Part III

1) A. de Shalit and I. Talmi, Nuclear Shell Theory (Academic Press, New York, 1963)

2) B. F. Bayman and A. Lande, Nuc. Phys. 77 (1966) 1

3) A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. 124 (1961) 162

4) R. Arvieu and S. A. Moszkowski, Phys. Rev. 145 (1966) 830

5) N. Newby, Jr. and E. J. Konopinski, Phys. Rev. 115 (1959) 434

6) A. Plastino, R. Arvieu, and S. A. Moszkowski, Phys. Rev. 145 (1966) 837

7) N. Auerbach, Nuc. Phys. 76 (1966) 321
   - - - , Phys. Lett. 21 (1966) 57

8) S. Cohen, R. D. Lawson, M. H. Macfarlane, S. P. Pandya, and M. Soga, Phys. Rev. 160 (1967) 903

9) L. S. Kisslinger and R. A. Sorensen, Rev. Mod. Phys. 35 (1963) 853; 36 (1964) 1104

10) E. L. Church and J. Weneser, Phys. Rev. 103 (1956) 1035

11) S. G. Nilsson, Mat. Fys. Medd. Dan. Vid. Selsk. 29, No. 16 (1955)

12) L. A. Koneg, J. H. E. Mattauch, and A. H. Wapstra, Nuc. Phys. 31 (1962) 18

13) C. D. Kavaloski, J. S. Lilley, D. C. Shreve, N. Stein, Phys. Rev. 161 (1967) 1107

14) C. M. Lederer, J. M. Hollander, and I. Perlman, Table of Isotopes, Sixth Edition (John Wiley and Sons, New York, 1967)

15) R. M. Kloepper, R. B. Day, and D. A. Lind, Phys, Rev. 114 (1959) 240

16) R. L. Graham and J. S. Geiger, private communication. P. Salling, Nuc. Phys. 65 (1965) 520

17) S. G. Nilsson and O. Prior, Mat. Fys. Medd. Dan. Vid. Selsk. 32, No. 16 (1967)

18) O. Bohigas, C. Quesne, and R. Arvieu, Phys. Lett. 26B (1968) 562

19) A. R. Edmonds, Angular Momentum in Quantum Mechanics, Second Edition (Princeton University Press, Princeton, N. J., 1960)

20) A. Bohr and B. R. Mottelson, Nuclear Structure and Energy Spectra, to be published.

21) A. Messiah, Quantum Mechanics, Vol. I (North-Holland Publishing Co., Amsterdam, 1966) p. 483

22) K. W. Ford and E. J. Konopinski, Nuc. Phys. 9 (1958/59) 218

23) K. Kumar and M. Baranger, Nuc. Phys. A92 (1967) 608, Section 4.2

GENERAL CONCLUSIONS

Parts I and II of this thesis dealt with the general problem of adapting the quasi-particle approximation to give satisfactory results in nuclear systems. Part I showed that the projection of correct particle number from the number non-conserving quasi-particle ground state vector can give excellent agreement with exact ground states, when the quasi-particle ground state is first modified by an exponential four, eight, etc , quasi-particle operator.

The similarity of this ground state exponential form to that predicted by the quasi-boson method led to Part II, which considers the generalized problem of computing both ground and excited seniority zero 0+ states of nuclei. The results of Part II demonstrate that, with the modifications discussed in the conclusion of Part II (section (9), excellent overlap of boson and exact 0+ states is obtained, especially if the number non-conservation problem is overcome by projection of exact particle number from the quasi-boson states.

One of the consequences of the modifications of the quasi-boson method and precautions for its use developed in Part II is that, for deformed nuclei, the β vibrational states can now be calculated, even for weak pairing, with greater confidence that the energies and state vectors obtained are valid. This result is important in deformed systems where the dimension of configuration space is so great as to require an approximation such as the quasi-particle, quasi-boson one.

For nuclear systems in which j-j coupling is appropriate (non-deformed systems), the results of Part II serve to complete the quasi-boson (RPA) program, which is generally accepted already to give good approximate energies for J = 0 states of seniority two in even nuclei. The results of Part II demonstrate that, when applied with the suggested modifications, the quasi-boson (RPA) method also is a valid approximation for first excited seniority zero 0+ states. In general, of course, all of the quasi-particle methods are number non-conserving, and should properly be followed by number projection.

The fact that the solution of the quasi-particle equations, plus solution of the quasi-boson equations, plus projection of correct particle number, plus re-calculation of energies with the projected state vectors, is a fairly complex computer problem, leads to the suggestion made in Part III of this thesis. We suggest there that for non-deformed nuclear systems, the method of exact, number conserving diagonalization of the many body Hamiltonian matrix has much to recommend it. The exact method is conceptually simpler than the quasi-particle method. The results obtained are linked directly to the physical assumptions made (single particle energies, form of residual potential, etc.). This simplicity is a contrast to the quasi-particle method, in which a great deal of effort must go into the isolation and correction of approximation

produced inaccuracies.

To illustrate, the study in section 5 of Part III of the isotopes of Ni shows that a certain single particle energy parameterization with a certain residual potential gives a reasonable fit to seniority zero and one excitation energies. If we had used the quasi-particle method in this study, however, the problem of number non-conservation would have introduced into our results an averaging of properties over several neighboring isotopes. The exact meaning of quasi-particle energies, for example, is therefore not so clear as the meaning of the energies which we obtained. Methods, such as the inverse gap equations, etc., which identify the experimental energies as quasi-particle energies seem to involve this difficulty of interpretation.

On the other hand, suppose that we had projected correct particle number from the quasi-particle states. We would then have needed to calculate the many body Hamiltonian matrix in order to re-calculate the excitation energies. It seems, however, that if we are going to calculate this Hamiltonian, we may as well diagonalize it directly, unless it is too large.

We conclude that the quasi-particle method is really only appropriate for those systems which have too large a number of configurations to allow direct diagonalization of the many body Hamiltonian. For most j-j coupled systems, direct diagonalization in seniority truncated spaces seems

the most direct and practical way to proceed. This is so certainly for states of seniority zero and one, since the calculation of the many body Hamiltonian is quite simple and easy to automate in these cases. Progress in computer technology, allowing larger matrices to be diagonalized in short times, and the development of simple methods for seniority two states, similar to the ones used here for seniority zero and one, should eventually cause exact, number conserving methods to replace quasi-particle methods for shell model calculations in non-deformed nuclear systems.

APPENDICES

Appendix III-A

Wave Functions and Radial Integrals

Single particle j-j coupling wave function:

$$\varphi_{n\ell jm}(\bar{r}) = \langle \bar{r} | n\ell jm \rangle$$

$$= \frac{1}{r} R_{n\ell}(r) \sum_{sq} \langle \tfrac{1}{2} s\, \ell q | j m \rangle \chi^{\frac{1}{2}}_{s}\; i^{\ell}\, Y^{\ell}_{q}(\hat{r}) \qquad (1)$$

where

$$r = |\bar{r}| \quad , \qquad \hat{r} = \frac{\bar{r}}{r}$$

The Pauli spin vector, $\chi^{1/2}_{s}$, has azimuthal spin component, s. The spherical harmonics $Y^{\ell}_{q}(\hat{r})$ have the standard phases (see, e.g., ref.[19]). The $R_{n\ell}(r)$ is the radial wave function defined below (eq. (9)).

Symmetries:

$$P\, \varphi_{n\ell jm}(\bar{r}) = (-1)^{\ell}\, \varphi_{n\ell jm}(\bar{r}) \qquad (2)$$

References in these Appendices are found in: References to Part III.

$$\vec{T}\,\varphi_{n\ell jm}(\bar{r}) = (-1)^{j-m}\,\varphi_{n\ell j-m}(\bar{r})$$

$$R_{\pi}\,\varphi_{n\ell jm}(\bar{r}) = (-1)^{j-m}\,\varphi_{n\ell j-m}(\bar{r}) \qquad (2)$$

where P, $\vec{T}$, and R_{π} are, respectively, parity, time reversal, and rotation by 180° about the y-axis. Then $R_{\pi}^{-1}\,T$ is anti-unitary operator with

$$R_{\pi}^{-1}\,\vec{T}\,\varphi_{n\ell jm}(\bar{r}) = \varphi_{n\ell jm}(\bar{r}) \qquad (3)$$

Reality of matrix elements:

If $[Q\,;\,R_{\pi}^{-1}\vec{T}] = 0$, and $Q^{+} = Q$, then

$$\langle j'm'|Q|jm\rangle = \langle j'm'|(R_{\pi}^{-1}\vec{T})^{-1}Q(R_{\pi}^{-1}\vec{T})|jm\rangle$$

$$= \langle j'm'|Q|jm\rangle^{*} \qquad (4)$$

Also, if Q anti-commutes with $R_{\pi}^{-1}\,T$, then the matrix element is pure imaginary.

Relation to usual convention (e.g., as given by de Shalit and Talmi[1]) and labeled "ST" below):

$$\varphi_{n\ell jm} = i^{\ell}\,\varphi_{n\ell jm}^{(ST)} \qquad (5)$$

$$|j_1^{\nu_1} j_2^{\nu_2} \cdots\rangle = (i)^{\nu_1 \ell_1 + \nu_2 \ell_2 + \cdots} |j_1^{\nu_1} j_2^{\nu_2} \cdots\rangle^{(ST)} \tag{7}$$

If all ν's are even, $p_k = \frac{1}{2}\nu_k$,

$$|j_1^{2p_1} j_2^{2p_2} \cdots\rangle = (-1)^{p_1 \ell_1 + p_2 \ell_2 + \cdots} |j_1^{2p_1} j_2^{2p_2} \cdots\rangle^{(ST)} \tag{8}$$

If all the ν's are even, plus one particle in state s, the right hand side of the previous equation (eq. (8)) should be multiplied by $(i)^{\ell_s}$. If all ℓ's but ℓ_a are even,

$$(-1)^{p_1 \ell_1 + p_2 \ell_2 + \cdots} = (-1)^{p_a}$$

If all ℓ's but ℓ_a are odd

$$(-1)^{p_1 \ell_1 + p_2 \ell_2 + \cdots} = (-1)^{p} (-1)^{p_a}$$

where p is the total number of pairs.

Radial wave function (harmonic oscillator):

$$R_{n\ell}(r) = N_{n\ell}\, e^{-\frac{1}{2}\rho^2} \rho^{\ell+1} L_{n-1}^{\ell+1/2}(\rho^2) \tag{9}$$

where $\rho = r/b$, $b = (\hbar/M\omega)^{1/2}$. The parameter

$\hbar\omega$ is chosen to give roughly the correct rms nuclear radius[11]),

$$\hbar\omega = 41\, A^{-1/3} \text{ MeV} .$$

The parameter, M, is the nucleon mass.

$$N_{n\ell} = \left\{ \frac{2(n-1)!}{b\left[\Gamma(n+\ell+1/2)\right]^3} \right\}^{1/2} \tag{10}$$

The notation for the associated Laguerre polynomial, L, is that of ref[21]). Thus

$$R_{1\ell}(r) = \left\{ \frac{2^{\ell+2}}{b\sqrt{\pi}\,(2\ell+1)!!} \right\}^{1/2} e^{-\frac{1}{2}\rho^2}\, \rho^{\ell+1}$$

$$R_{2\ell}(r) = R_{1\ell}(r)\, \frac{(\ell+3/2) - \rho^2}{(\ell+3/2)^{1/2}} \tag{11}$$

$$R_{3\ell}(r) = R_{1\ell}(r)\, \frac{(\ell+5/2)(\ell+3/2) - 2\rho^2(\ell+5/2) + \rho^4}{\left[2(\ell+5/2)(\ell+3/2)\right]^{1/2}}$$

where

$$(2\ell+1)!! = (2\ell+1)(2\ell-1)(2\ell-3)\cdots 1 .$$

Eqs. (11) agree with those of ref.[5]).

Radial integrals of delta potential:

$$I_{ijij} = \frac{1}{4\pi}\int_0^\infty \frac{dr}{r^2}\left[R_{n_i\ell_i}(r)\right]^2 \left[R_{n_j\ell_j}(r)\right]^2$$

can be expressed as a sum of integrals of a standard form

(e.g., see ref.[22]),

$$f_k(m,m') = \frac{1}{2k+1}\iint \rho_1^2\, d\rho_1\, \rho_2^2\, d\rho_2\, \rho_1^m\, \rho_2^{m'}\, e^{-\rho_1^2-\rho_2^2}\, v_k(b\rho_1, b\rho_2) \tag{13}$$

with

$$v_k(r_1,r_2) = \frac{2k+1}{2}\int_{-1}^{+1} d(\cos\Theta_{12})\, P_k(\cos\Theta_{12})\, V(|\bar{r}_1-\bar{r}_2|) \quad .$$

Then

$$V(|\bar{r}_1-\bar{r}_2|) = -V_\delta\, \delta(\bar{r}_1-\bar{r}_2) = -V_\delta \frac{\delta(r_1-r_2)}{r_1 r_2}\, \delta(\cos\Theta_1-\cos\Theta_2)\frac{1}{2\pi} \tag{14}$$

gives

$$v_k(r_1,r_2) = -V_\delta \frac{2k+1}{4\pi}\, \frac{\delta(r_1-r_2)}{r_1 r_2} \tag{15}$$

and

$$f_k(m,m') = \frac{-V_\delta}{4\pi b^3}\int_0^\infty d\rho\, \rho^{m+m'+2}\, e^{-2\rho^2} \tag{16}$$

which does not depend on index k, and which is an easily evaluated standard integral. A computer program which evaluates eq. (12) using eqs. (11) and (16) is listed in Appendix III-E.

Appendix III-B

Commutation Relations of Operators

Definitions:

$$a^{+}_{ij}(JM) = \sum_{qm} \langle i q j m | J M \rangle \, c^{+}_{iq} \, c^{+}_{jm}$$

$$n_{ij}(JM) = -\sum_{qm} \langle i q j m | J M \rangle \, c^{+}_{iq} \, (-1)^{j-m} c_{j\,-m} \qquad (1)$$

Symmetries:

$$a^{+}_{ji}(JM) = (-1)^{i-j+J} \, a^{+}_{ij}(JM)$$

$$n_{ji}(JM) = (-1)^{i-j+J} (-1)^{J-M} \, n^{+}_{ij}(J\,-M) \qquad (2)$$

Commutation relations:

$$[a_{ij}(JM), a^{+}_{rs}(J'M')] = \delta_{JJ'}\delta_{MM'}\left(\delta_{ir}\delta_{js} + (-1)^{i-j+J}\delta_{is}\delta_{jr}\right)$$

$$+ \left[(2J+1)(2J'+1)\right]^{1/2} (-1)^{J-M} \sum_{K=|J-J'|}^{J+J'} \langle J\,-M\;J'\,M' | K\mu \rangle \times$$

$$\times \Bigg[\delta_{ir} (-1)^{i-j+J} \begin{Bmatrix} J & j & i \\ s & J' & K \end{Bmatrix} n_{sj}(K\mu) \qquad (3)$$

$$+ \delta_{jr} \begin{Bmatrix} J & i & j \\ s & J' & K \end{Bmatrix} n_{si}(K\mu) \tag{3}$$

$$+ \delta_{is} (-1)^{i-j+J} (-1)^{r-s+J'} \begin{Bmatrix} J & j & i \\ r & J' & K \end{Bmatrix} n_{rj}(K\mu)$$

$$+ \delta_{js} (-1)^{r-s+J'} \begin{Bmatrix} J & i & j \\ r & J' & K \end{Bmatrix} n_{ri}(K\mu) \Bigg]$$

$$[n_{ij}(JM), a^{+}_{rs}(J'M')] = -\left[(2J+1)(2J'+1)\right]^{\frac{1}{2}} \sum_{K=|J-J'|}^{J+J'} \langle JMJ'M'|K\mu\rangle \times$$

$$\times \Bigg[\delta_{jr} \begin{Bmatrix} J & i & j \\ s & J' & K \end{Bmatrix} a^{+}_{si}(K\mu) \tag{4}$$

$$+ \delta_{sj} (-1)^{r-s+J'} \begin{Bmatrix} J & i & j \\ r & J' & K \end{Bmatrix} a^{+}_{ri}(K\mu) \Bigg]$$

$$[n_{ij}(JM), n_{rs}(J'M')] = [(2J+1)(2J'+1)]^{1/2} \times \tag{5}$$

$$\times \sum_{K=|J-J'|}^{J+J'} \Big[\delta_{is} \langle J'M'JM|K\mu\rangle \begin{Bmatrix} J & j & i \\ r & J' & K \end{Bmatrix} (-1)^{r-j+K} n_{rj}(K\mu)$$

$$- \delta_{jr} \langle JMJ'M'|K\mu\rangle \begin{Bmatrix} J & i & j \\ s & J' & K \end{Bmatrix} (-1)^{i-s+K} n_{is}(K\mu) \Big]$$

$$[n_{rs}(JM), c^{+}_{jm}] = \delta_{sj} (-1)^{j-m} \langle r\mu\, j\, -m|JM\rangle c^{+}_{r\mu} \tag{6}$$

$$[a_{rs}(JM), c^{+}_{jm}] = \delta_{rj} \langle j\, m\, s\mu|JM\rangle C_{s\mu} \tag{7}$$

$$- \delta_{sj} \langle r\mu\, j\, m|JM\rangle C_{r\mu}$$

The above relations are derived using the anti-commutation relations of the c^{+}_{jm} operators

$$c_{iq} c^{+}_{jm} + c^{+}_{jm} c_{iq} = \delta_{ij} \delta_{qm}$$

$$c^{+}_{iq} c^{+}_{jm} + c^{+}_{jm} c^{+}_{iq} = 0$$

and the relations for vector coupling coefficients and for 6-j symbols (curly brackets above) given on pp. 40-42 and pp. 95-98 of ref.[19]). The value of η above is in each case determined from the conservation of total azimuthal quantum number implicit in the definition of the vector coupling coefficients.

Simple special cases:

Suppose i = j = r = s and J' = 0 in eqs. (1)-(7). Then

$$[a_{jj}(JM), a^{+}_{jj}(00)] = 2\delta_{J0} - \frac{4}{\sqrt{(2j+1)}}(-1)^{J-M} n_{jj}(J-M) \tag{11}$$

$$[n_{jj}(JM), a^{+}_{jj}(00) = \frac{2}{\sqrt{(2j+1)}} a^{+}_{jj}(JM) \tag{12}$$

$$[n_{jj}(JM), n_{jj}(00)] = 0 \tag{13}$$

If, also, J = 0, define

$$a^{+}_{j} = \frac{1}{\sqrt{2}} a^{+}_{jj}(00) \tag{14}$$

and note that

$$n_{jj}(00) = \frac{1}{\sqrt{(2j+1)}} n_j \tag{15}$$

where

$$n_j = \sum_m c^+_{jm} c_{jm} \quad . \tag{16}$$

Then

$$[a_i, a_j^+] = \delta_{ij}\left(1 - \frac{1}{\Omega_j} n_j\right),$$

$$[n_i, a_j^+] = 2\delta_{ij} a_j^+ \quad , \tag{17}$$

where

$$\Omega_j = \frac{1}{2}(2j+1) \quad .$$

Appendix III-C

Many Particle States Defined

Seniority zero states: p pairs.

$$a_j^+ = \frac{1}{\sqrt{2}} a_{jj}^+ (0\,0)$$

$$|p_j\rangle = \mathcal{N}_j^{-1}(p) \, (a_j^+)^p \, |0\rangle$$

$$\mathcal{N}_j^2(p) = \langle 0| (a_j)^p (a_j^+)^p |0\rangle = \frac{(p!)^2}{\Omega_j^p} \binom{\Omega_j}{p}$$

$$a_j^+ |p_j\rangle = \left[\frac{(p+1)(\Omega_j - p)}{\Omega_j} \right]^{1/2} |(p+1)_j\rangle$$

Seniority one states: p pairs plus one particle.

$$|\overline{p_j}\rangle = \bar{\mathcal{N}}_j^{-1}(p) \, (a_j^+)^p \, c_{jm}^+ \, |0\rangle$$

$$\bar{\mathcal{N}}_j^2(p) = \langle 0| c_{jm} (a_j)^p (a_j^+)^p c_{jm}^+ |0\rangle$$

$$= \frac{(p!)^2}{\Omega_j^p} \binom{\Omega_j}{p} \frac{\Omega_j - p}{\Omega_j}$$

$$a_j^+ |\overline{p_j}\rangle = \left[\frac{(p+1)(\Omega_j - p - 1)}{\Omega_j} \right]^{1/2} |\overline{(p+1)_j}\rangle$$

Seniority two states: p pairs plus two particles.

$$|\overline{\overline{P_j}}\rangle = \overline{\overline{\mathcal{N}}}_j^{-1}(p)\,(a_j^+)^p \frac{1}{\sqrt{2}}\, a_{jj}^+(JM)\,|0\rangle\,, \qquad J \neq 0$$

$$\overline{\overline{\mathcal{N}}}_j^{2}(p) = \frac{1}{2}\langle 0|\, a_{jj}(JM)\,(a_j)^p\,(a_j^+)^p\, a_{jj}^+(JM)\,|0\rangle$$

$$= \frac{(p!)^2}{\Omega_j^p}\binom{\Omega_j}{p}\frac{(\Omega_j-p)(\Omega_j-p-1)}{\Omega_j(\Omega_j-1)}$$

$$a_j^+\,|\overline{\overline{P_j}}\rangle = \left[\frac{(p+1)(\Omega_j-p-2)}{\Omega_j}\right]^{\frac{1}{2}} |\overline{\overline{(p+1)_j}}\rangle$$

$$\frac{1}{\sqrt{2}}\, a_{jj}^+(JM)\,|P_j\rangle = \left[\frac{(\Omega_j-p)(\Omega_j-p-1)}{\Omega_j(\Omega_j-1)}\right]^{1/2} |\overline{\overline{P_j}}\rangle$$

Seniority two states: p pairs plus one particle and q pairs plus one particle.

$$|\overline{P_i\, q_j}\rangle = \overline{\mathcal{N}}_{ij}^{-1}(pq)\,(a_i^+)^p\,(a_j^+)^q\, a_{ij}^+(JM)\,|0\rangle$$

$$\overline{\mathcal{N}}_{ij}^{2}(pq) = \langle 0|\, a_{ij}(JM)\,(a_j)^q\,(a_i)^p\,(a_i^+)^p\,(a_j^+)^q\, a_{ij}^+(JM)\,|0\rangle$$

$$= \frac{(p!)^2}{\Omega_i^p}\binom{\Omega_i}{p}\frac{(q!)^2}{\Omega_j^q}\binom{\Omega_j}{q}\frac{\Omega_i-p}{\Omega_i}\,\frac{\Omega_j-q}{\Omega_j}\,.$$

Appendix III-D

Many Particle Matrix Elements for Seniority Zero and One

Using notation from Appendix III-C preceeding:

$$\langle p_j | a_j^+ a_j | p_j \rangle = \frac{p(\Omega_j - p + 1)}{\Omega_j} \tag{1}$$

$$\langle (p+1)_i \, (q-1)_j | a_i^+ a_j | p_i \, q_j \rangle$$

$$= \left[\frac{(p+1)(\Omega_i - p)}{\Omega_i} \quad \frac{q(\Omega_j - q + 1)}{\Omega_j} \right]^{\frac{1}{2}} \tag{2}$$

$$\langle \bar{p}_j | a_j^+ a_j | \bar{p}_j \rangle = \frac{p(\Omega_j - p)}{\Omega_j} \tag{3}$$

$$\langle \overline{(p+1)}_i \, (q-1)_j | a_i^+ a_j | \bar{p}_i \, q_j \rangle \tag{4}$$

$$= \left[\frac{(p+1)(\Omega_i - p - 1)}{\Omega_i} \quad \frac{q(\Omega_j - q + 1)}{\Omega_j} \right]^{1/2}$$

$$\langle (p+1)_i \, \overline{(q-1)}_j | a_i^+ a_j | p_i \, \bar{q}_j \rangle \tag{5}$$

$$= \left[\frac{(p+1)(\Omega_i - p)}{\Omega_i} \quad \frac{q(\Omega_j - q)}{\Omega_j} \right]^{1/2}$$

$$\langle p_j | a_{jj}^+ (JM) \, a_{jj} (JM) | p_j \rangle = \frac{2p(p-1)}{\Omega_j(\Omega_j - 1)} \tag{6}$$

$$\langle \bar{p}_j | a^{+}_{jj}(JM)\, a_{jj}(JM) | \bar{p}_j \rangle = \frac{2p^2}{\Omega_j(\Omega_j - 1)} \qquad (7)$$

$$\langle p_i q_j | a^{+}_{ij}(JM)\, a_{ij}(JM) | p_i q_j \rangle = \frac{p}{\Omega_i} \frac{q}{\Omega_j} \qquad (8)$$

$$\langle \bar{p}_i q_j | a^{+}_{ij}(JM)\, a_{ij}(JM) | \bar{p}_i q_j \rangle = \frac{p + \frac{1}{2}}{\Omega_i} \frac{q}{\Omega_j} \qquad (9)$$

Eqs. (1)-(8) above are derived from commutation relations in Appendix III-B and the states defined in Appendix III-C. Use is made of the relations on pp. 40-42 and pp. 95-98 of ref.[19]). Eqs. (1), (3), (6), and (7) above, when inserted in eq. (19) of Part III, agree with the interaction energies in states with lowest seniority given on p. 533 of ref.[1]). (Note that the two body matrix elements in ref.[1]) are one-half times our G(ijijJ) expressions.)

Appendix III-E

Computer Programs

1. PROGRAM TET computes and diagonalizes the many body Hamiltonian matrix of a general potential in seniority zero and one spaces.

2. SUBROUTINE CONFIG is called by TET to compute the configurations of NPR pairs in LEVELS number of j-levels, with the pair multiplicities MULT(J) and seniorities ISEN(J).

3. FORTRAN IV SUBROUTINE MEERA-ORTHO computes the first four eigen vectors and eigen values of the many body Hamiltonian matrix of dimension LEV. This program was written by K. Kumar[23]) and provided by him to the nuclear structure group at Berkeley.

4. SUBROUTINE SKEPTIC checks the eigen vectors and values from MEERA-ORTHO by forming the vector

$$r_k^{(a)} = \frac{1}{E^{(a)}}\left(\sum_m H_{km}\,\phi_m^{(a)} - E^{(a)}\,\phi_k^{(a)}\right)$$

for each root, a, using eigen energies $E^{(a)}$ and eigen vectors $\phi_k^{(a)}$. It then forms and prints

$$\left(\sum_k (r_k^{(a)})^2\right)^{1/2}, \quad \sum_k |r_k^{(a)}|, \quad r_k^{(a)}/\phi_k^{(a)}$$

which should all be small if the eigen solution is valid.

5. SUBROUTINE EZERO calculates the rho-square of the $E^*_{0+} \dashrightarrow E_{0+}$ transition for proton systems using eigen vectors from TET. Parameters A, L(J), N(J) must be set

to the atomic number of the nucleus, the orbital angular momentum of the j-levels, and the oscillator quantum number of the j-levels, respectively.

6. PROGRAM SLATER computes radial integrals of a delta potential using harmonic oscillator wave functions. The parameters A, L(J), N(J) must be set as in EZERO above.

7. FUNCTION RADIAL is called by SLATER to compute radial integrals for a given set of four j-levels.

8. FUNCTION FFF is called by RADIAL to compute the $f_k(m,m')$ function given in eq. (13) of Appendix III-A.

9. PROGRAM TRANONE reads punched output of TET and computes the spectroscopic factors of one nucleon transfer reactions.

```
      PROGRAM TET (INPUT,OUTPUT,TAPE3=OUTPUT,PUNCH)
C SENIORITY ZERO 0+ SPECTRUM AND SENIORITY ONE SPECTRUM
C BY EXACT DIAGONALIZATION OF A GENERAL POTENTIAL
C LEVELS IS THE NUMBER OF SHELL-MODEL LEVELS
C NPR IS THE NUMBER OF PAIRS
C LEV IS THE NUMBER OF CONFIGURATIONS
C MH IS NUMBER OF NONZERO SUPER-DIAGONAL ELEMENTS OF H

C DIMENSION ARRAYS AS FOLLOWS......
C IX(LEVELS,LEV),Z(LEVELS),MULT(LEVELS),S(LEVELS,LEVELS),OC(LEVELS)
C QP(LEVELS),E(4),R(4),W(LEV,4),H(MH),IH(MH),JH(MH),ZL(LEVELS)
C DEL(LEVELS),S2(LEVELS,LEVELS),ISEN(LEVELS),NULT(LEVELS),OD(LEVELS)
      DIMENSION P(10,10),Q(10,10),Z(10),OC(10),S(10,10),QP(10),S2(10,10)
      DIMENSION H(1275),E(4),W(200,4),     IH(1275),JH(1275),R(4)
      DIMENSION MULT(10),IX(10,200),ZL(10),DEL(10),ISEN(10),NULT(10)
      DIMENSION OD(10)

C FOR NO PUNCHED OUTPUT, SET IPUNCH=0
C TO PUNCH ONLY E-VALUES AND E-VECTORS, SET IPUNCH=1
C TO PUNCH H, E-VALUES, AND E-VECTORS, SET IPUNCH=2
      IPUNCH=0
C SET NCARD=NUMBER OF NUCLEI TO BE RUN
      NCARD=17
C SET IS=0 IF WISH TO READ-IN S VALUES.  =2 IF WISH ALL S=-1.
      IS=2
C SET IS2=0 IF WISH TO READ-IN S2 VALUES.  =2 IF WISH ALL S2=0.
C SET IS2=1 IF WISH S2 DERIVED FROM S AS IN A DELTA-POTENTIAL
C FOR A SURFACE-DELTA POTENTIAL, IS=2 AND IS2=1 .
      IS2=1
C E-VALUES WILL BE ACCURATE TO ABOUT H0 TIMES THEIR MAGNITUDES.
      H0=1.0E-14
C THE PROGRAM WILL COMPUTE THE FIRST IP3 E-VECTORS.
      IP3=4


    1 FORMAT(16I5)
    2 FORMAT (10F8.5)
C READ-IN THE NUMBER OF J-LEVELS
      READ 1, LEVELS
C READ-IN PAIR MULTIPLICITIES OF J-LEVELS
      READ 1, (MULT(I),I=1,LEVELS)
      DO 4 I=1,LEVELS
      DO 4 J=1,LEVELS
      S2(I,J)=0.
    4 S(I,J)=-1.
      IF(IS.GT.1)GO TO 55
C IF IS=0, READ-IN S(I,J) S.T.
C G*S(I,J)=+(II,0/V/JJ,0)/SQRT((2J+1)*(2I+1)).
      DO 5 I=1,LEVELS
      READ 2,(S(I,J),J=1,I)
      DO 5 J=1,I
```

```
    5 S(J,I)=S(I,J)
   55 CONTINUE
      SI2=IS2
      IF(SI2.GT.0.1) GO TO 56
C IF IS2=0, READ-IN S2(I,J) SUCH THAT
C   G*S2(I,J)= $SUM OVER K$ (2K+1)*(IJ,K/V/IJ,K).
      DO 6, I=1,LEVELS
      READ 2, (S2(I,J),J=1,I)
      DO 6  J=1,I
    6 S2(J,I)=S2(I,J)
   56 CONTINUE
      SI2=(SI2-1.)**2
      IF(SI2.GT.0.1) GO TO 54
      DO 51 I=1,LEVELS
      DO 51 J=1,LEVELS
      D=0.
      R=I-J
      IF(R**2.LT.0.1) D=1.
      OI=MULT(I)
      OJ=MULT(J)
   51 S2(I,J)=2.*(OI-D)*OJ*S(I,J)
   54 CONTINUE

      DO 3 IA=1,NCARD
C READ-IN THE NUMBER OF PAIRS
      READ 1, NPR
C READ-IN SINGLE PARTICLE ENERGIES OF J-LEVELS
      READ 2, (Z(I),I=1,LEVELS)
C READ-IN THE SENIORITIES OF THE J-LEVELS
      READ 1, (ISEN(I),I=1,LEVELS)
      DO 7  I=1,LEVELS
    7 NULT(I)=MULT(I)-ISEN(I)

      CALL CONFIG(NPR,LEVELS,LEV,NULT,IX)

C SET NG=NUMBER OF G-VALUES TO BE RUN
      NG=1
C IF NGREAD=0, THEN READ-IN THE DIFFERENT G-VALUES
C IF NGREAD=2, START AT G=GO AND ITERATE BY GIT FOR NG TIMES
      NGREAD=2
      GO=0.45
      GIT=0.1

      G=GO
      DO 8 IG=1,NG
      IF(NGREAD.LT.1)READ 9, G
    9 FORMAT(5E15.6)
      DO 11 I=1,4
      E(I)=0.
      R(I)=0.
      DO 11 J=1,LEV
   11 W(J,I)=0.
      MH=0
      DO 13 J=1,LEV
      DO 13 JJ=1,LEV
```

```
C   IS JJ EQUAL TO J
      R=JJ-J
      IF(R**2.GT.0.1) GO TO 14
C   IF SO, CALCULATE DIAGONAL MATRIX ELEMENT
      B=0.
      DO 15 I=1,LEVELS
      O=MULT(I)
      SEN=ISEN(I)
      X=IX(I,J)
      OH=O*(O-1.)
      IF(O.LT.1.1)OH=1.
      B=B+Z(I)*(2.*X     )+G*S(I,I)*X*(O-X+1.-SEN)
      B=B+0.5*G*S2(I,I)*X*(X-1.+SEN)/OH
      DO 15 K=1,I
      R=I-K
      IF(R.LT.0.5)GO TO 15
      SENK=ISEN(K)
      OK=MULT(K)
      Y=IX(K,J)
      B=B+G*S2(I,K)*(X+0.5*SEN)*(Y+0.5*SENK)/(O*OK)
   15 CONTINUE
      GO TO 16
C   IF NOT, IS JJ GREATER THAN J
   14 R=JJ-J
      IF(R.LT.(-0.1)) GO TO 13
C   IF IT IS, CALCULATE NON-DIAGONAL MATRIX ELEMENT
      B=0.
      ATEST=0.
      DO 17 I=1,LEVELS
      X=IX(I,J)
      XX=IX(I,JJ)
   17 ATEST=ATEST+(X-XX)**2
      IF(ATEST.GT.0.1) GO TO 18
      PRINT 19
   19 FORMAT(/* TWO CONFIGURATIONS ARE THE SAME*)
      GO TO 8
   18 ATEST=ATEST-2.
      IF(ATEST**2.GT.0.1)GO TO 13
      DO 30 I=1,LEVELS
      DO 30 N=1,LEVELS
      X=IX(I,J)
      XX=IX(I,JJ)
      Y=IX(N,J)
      YY=IX(N,JJ)
      R=(X-XX-1.)**2+(Y-YY+1.)**2
      IF(R.GT.0.1) GO TO 30
      ON=MULT(N)-ISEN(N)
      OI=MULT(I)-ISEN(I)
      R=(XX+1.)*(OI-XX)*YY*(ON-YY+1.)
      IF(R.GT.0.)B=B+SQRT(R)*G*S(I,N)
   30 CONTINUE
C   IF MATRIX ELEMENT IS NON-ZERO, ENTER IT IN H
   16 IF(B.EQ.0.) GO TO 13
      MH=MH+1
      IH(MH)=J
```

```
      JH(MH)=JJ
      H(MH)=B
   13 CONTINUE
      IT=0
      M=LEV
      M1=M
      CALL MEERA(H0,IP3,IT,H,E,W,IH,JH,R,M,M1,MH)
      PRINT 23,LEVELS,LEV,G
   23 FORMAT(//* THE NUMBER OF LEVELS IS*,I5,32H THE NUMBER OF CONFIGURA
     1TIONS IS,I5, 9H AND G IS,E15.5)
      PRINT 24, (MULT(I),I=1,LEVELS)
   24 FORMAT (//34H PAIR MULTIPLICITIES OF LEVELS ARE,10I5)
      PRINT 26
   26 FORMAT (/* THE S(I,J) ARE*)
      REVELS=LEVELS
      DO 27 I=1,LEVELS
      PRINT28, (S(I,J),J=1,LEVELS)
      R=MULT(I)-ISEN(I)
      IF(R.LT.0.1) REVELS=REVELS-1.
   27 CONTINUE
   28 FORMAT(/10F10.5)
      PRINT 52
   52 FORMAT(/* THE S2(I,J) ARE*)
      DO 53 I=1,LEVELS
      PRINT 28, (S2(I,J),J=1,LEVELS)
   53 CONTINUE
      PRINT 10
   10 FORMAT(/* THE MATRIX H(I,J), WITHOUT ODD-PART. ENERGY, IS*/)
      PRINT 20,  (H(K),IH(K),JH(K),K=1,MH)
   20 FORMAT (4(E20.8,2H (,I3,I4,1H)))
      PU=IPUNCH
      IF(PU.GT.1.5)  PUNCH 21,(H(K),IH(K),JH(K),K=1,MH)
   21 FORMAT(4(E14.7,2I3))
      PRINT 22, MH
   22 FORMAT (/9H THEREARE,I5,36H  NONZERO SUPER-DIAG MATRIX ELEMENTS//)
      PRINT 25, (Z(J),J=1,LEVELS)
   25 FORMAT(/* THE SP ENERGIES ARE*,10F9.5/)
      DO 57 I=1,4
      DO 57 J=1,LEVELS
      SEN=ISEN(J)
   57 E(I)=E(I)+SEN*Z(J)
      PU=IPUNCH
      IF(PU.GT.0.5) PUNCH 29, (E(I),I=1,4)
   29 FORMAT (5H EEEE,4E18.10)
      PRINT 31,  (E(I),I=1,4),(MULT(J),J=1,LEVELS)
   31 FORMAT(/* EIGEN-VALUES, INCLUDING ODD-PART. ENERGY, ARE*/4E20.10,1
     15X,10I3)
      PRINT 50, (ISEN(I),I=1,LEVELS)
   50 FORMAT(//* SENIORITIES OF THE J-LEVELS ARE...*,60X,10I3//)
      PRINT 32
   32 FORMAT (//18H EIGEN-VECTORS ARE)
      DO 33 K=1,LEV
      IF(PU.GT.0.5) PUNCH 34,K,(W(K,J),J=1,4),(IX(I,K),I=1,10)
   34 FORMAT(I4,4E16.7,2X,10I1)
      PRINT 35, (W(K,J),J=1,4), K,       (IX(I,K),I=1,LEVELS)
```

```
35 FORMAT(/4E20.10,5X,I5,5X,10I3)
33 CONTINUE
   PRINT 36, HO
36 FORMAT (//39H THE EIGEN-VALUES ARE ACCURATE TO ABOUT,E8.1,23H TIME
  1S THEIR MAGNITUDES)
   DO 37 I=2,4
37 E(I)=E(I)-E(1)
   E(1)=0.
   PRINT 38, (E(I),I=1,IP3)
38 FORMAT (/28H THE EXCITATION ENERGIES ARE/4E20.10)
   DO 39 I=1,LEVELS
   OC(I)=0.
   DO 40  K=1,LEV
   R=IX(I,K)
40 OC(I)=OC(I)+2.*R*W(K,1)**2
   SEN=ISEN(I)
   OD(I)=OC(I)+SEN
   R=MULT(I)-ISEN(I)
   IF(R.EQ.0.)R=1.0E-20
39 OC(I)=OC(I)/(2.*R)
   PRINT 58,(OD(I),I=1,LEVELS)
58 FORMAT(/* THE AVERAGE NOS. OF PARTICLES, (O/N/O), ARE*//10F11.6/)
   DO 59 I=1,LEVELS
   R=MULT(I)
59 OD(I)=OD(I)/(2.*R)
   PRINT 60,(OD(I),I=1,LEVELS)
60 FORMAT(/* THE OCCUPATION NOS., (O/N/O)/(2J+1), ARE*//10F11.6/)
   PRINT 41,  (OC(I),I=1,LEVELS)
41 FORMAT(/* THE  PAIR   OCCUPATION NUMBERS, V=(O/P/O)/(O-SEN), OF TH
  1E LEVELS ARE*//10F11.6/)
   ZLAM=0.
   DO 43 J=1,LEVELS
   DEL(J)=0.
   DO 44 I=1,LEVELS
   R=MULT(I)-ISEN(I)
   RR=1.-OC(I)
   IF(RR.LT.0.)RR=-RR
44 DEL(J)=DEL(J)-R*G*S(J,I)*SQRT(OC(I)*RR)
   RD=1.-2.*OC(J)
   RF=1.-RD**2
   IF(RF.LT.0.)RF=-RF
   IF(RF.EQ.0.)RF=1.0E-20
   ZL(J)=Z(J)-DEL(J)*RD/SQRT(RF)
   R=MULT(J)-ISEN(J)
   IF(R.LT.0.1) GO TO 43
   ZLAM=ZLAM+ZL(J)/REVELS
43 CONTINUE
   PRINT 45, (DEL(J),J=1,LEVELS)
45 FORMAT(/* THE DELTA(J) ARE*//8E15.6)
   PRINT 46, (ZL(J),J=1,LEVELS)
46 FORMAT(/* THE J-TH LEVEL APPROX. TO LAMBDA ARE*//8E15.6)
   PRINT 47, ZLAM
47 FORMAT(/* THE AVERAGE LAMBDA=*,E13.6)
   DO 48 I=1,LEVELS
48 QP(I)=SQRT((Z(I)-ZLAM)**2+DEL(I)**2)
```

```
      PRINT 49, (QP(I),I=1,LEVELS)
   49 FORMAT(/* THE Q.P. ENERGIES ARE*//1X,8E15.6)
      PRINT 42
   42 FORMAT (1H1)
      CALL EZERO(LEVELS,LEV,IX,W)
      G=G+GIT
    8 CONTINUE
    3 CONTINUE
      STOP
      END
      SUBROUTINE CONFIG(NPR,LEVELS,LEV,MULT,IX)
C DIMENSION ARRAYS SAME AS IN TET
      DIMENSION MULT(10),IX(10,200)
      DIMENSION II(10)
      II(1)=NPR
      DO 1  I=2,LEVELS
    1 II(I)=0
      KK=0
C  DOES THE CONFIG IN II EXCEED THE MULT OF ANY LEVEL
    2 DO 3 I=1,LEVELS
      R=MULT(I)-II(I)
      IF(R.LT.(-0.1))GO TO 4
    3 CONTINUE
C IF IT DOES NOT, THEN TRANSFER IT TO IX.
      KK=KK+1
      DO 5 I=1,LEVELS
    5 IX(I,KK)=II(I)
C  ARE WE FINISHED (IE., ALL ZEROES EXCEPT EXTREME RH ENTRY OF II)
    4 SUM=0.
      L=LEVELS-1
      DO 6 I=1,L
      R=II(I)
    6 SUM=SUM+R**2
      IF(SUM.GT.0.1) GO TO 7
      LEV=KK
      RETURN
C  IF NOT THEN SCAN II FROM RT FOR FIRST NON-ZERO, NON-EXTREME RH ENTRY
    7 DO 8 I=2,LEVELS
      J=LEVELS-I+1
      R=II(J)
      IF(R.GT.0.1) GO TO 9
    8 CONTINUE
C  HAVING FOUND A NON-ZERO ENTRY, REDUCE IT BY ONE
    9 II(J)=II(J)-1
C  THEN PUT THE REMAINING PAIRS IN THE NEXT ENTRY TO RIGHT AND PROCEED
      II(LEVELS)=0
      KSUM=0
      DO 10 I=1,J
   10 KSUM=KSUM+II(I)
      II(J+1)=NPR-KSUM
      GO TO 2
      END
      FORTRAN IV SUBROUTINE MEERA(HO,IP3,IT,H,E,W,IH,JH,R,M,M1,MH)
C
C     LOWEST FEW EIGEN-VALUES AND EIGEN-VECTORS
```

```
C
C DIMENSION ARRAYS SAME AS IN TET
      DIMENSION H(1275),E(4),W(200,4),IH(1275),JH(1275),R(4)
      COMMON X(200),SI(200),D(200),G(200)
  500 FORMAT(30I4)
  510 FORMAT(1X,7E17.9)
  230 EM=0.
      DO 10 I=1,M1
   10 EM=EM+1.
      EM=1./SQRT(EM)
      DO 126 IP= 1,IP3
      NI=0
      WP=1.E30
   20 I1=IP-1
      IF(IT)30,30,220
   30 DO 100 I=1,M
  100 X(I)=EM
  220 IF(I1)     120,120,117
  117 CALL ORTHO(I1,X,H,E,W,IH,JH,R,M,M1,MH)
  120 W1=0.
      T1=0.
      DO 101 I=1,M
  101 D(I)=0.
      DO 102 K=1,MH
      I=IH(K)
      J=JH(K)
      IF(J-I) 105,102,105
  105 D(J)=D(J)+H(K)*X(I)
  102 D(I)=D(I)+H(K)*X(J)
      DO 103 I=1,M
      IF(I-M1) 106,106,109
  106 G(I)=X(I)
      T1=T1+X(I)*G(I)
      GO TO 103
  109 SI(I)=D(I)
  103 W1=W1+X(I)*D(I)
      W3=W1/T1
      DO 110 I=1,M1
  110 SI(I)=D(I)-W3*G(I)
      SI2=0.
      DO 210 I=1,M
  210 SI2=SI2+SI(I)*SI(I)
      IF(SI2-1.E-12) 121,121,240
  240 X0=ABS(WP-W3)/(ABS(W3)+H0)
      IF(X0-H0) 121,121,70
   70 IF(I1) 111,111,128
  128 CALLORTHO(I1,SI,H,E,W,IH,JH,R,M,M1,MH)
  111 W2=0.
      NI=NI+1
      T2=0.
      Q =0.
      P =0.
      DO 115 I=1,M
      X0=SI(I)
      IF(I-M1) 104,104,115
```

```
  104 P=P+G(I)*X0
      T2=T2+X0*X0
  115 Q=Q+D(I)*X0
      DO 114 K=1,MH
      I=IH(K)
      J=JH(K)
      IF(J-I) 108,107,108
  107 X0=SI(I)*SI(I)
      GO TO 114
  108 X0=2.*SI(I)*SI(J)
  114 W2=W2+H(K)*X0
      C=T1*Q-W1*P
      B=0.5*(T1*W2-W1*T2)
      G1=C/(B+SQRT(B*B+C*(T2*Q-W2*P)))
      G1=G1*0.9
      DO 116 I=1,M
  116 X(I)=X(I)-G1*SI(I)
      WP=W3
      GO TO 120
C
  121 E(IP)=W3
      T=1./SQRT(T1)
      DO 122 I=1,M
      SI(I)=SI(I)*T
      X(I)=X(I)*T
  122 W(I,IP)=X(I)
      WRITE (3,830)NI
  830 FORMAT (4H NI=I4)
      IF(I1)  51,51,52
   52 CALL ORTHO(I1,X,H,E,W,IH,JH,R,M,M1,MH)
      WRITE(3,510)(R(I),I=1,I1)
      T=0.
      DO 11 I=1,M1
   11 T=T+SI(I)*SI(I)
      IF(T) 51,51,12
   12 T=1./SQRT(T)
      IT=1
      DO 13 I=1,M
   13 X(I)=SI(I)*T
   51 WRITE(3,510)W3
      WRITE (3,61)
   61 FORMAT (1H0)
  126 CONTINUE
      CALL SKEPTIC(H,IH,JH,E,W,MH,M)
      RETURN
      END
      FORTRAN IV SUBROUTINE ORTHO(I1,X,H,E,W,IH,JH,R,M,M1,MH)
C
C     ORTHOGONALIZATION TO ALL THE LOWER VECTORS
C
      DIMENSION H(1275),E(4),W(200,4),     IH(1275),JH(1275),R(4),X(200)
  201 FORMAT(  E14.6 )
  117 DO 119 IP1= 1,I1
      X0=0.
      DO 118 I=1,M1
```

```
  118 X0=X0+X(I)*W(I,IP1)
  119 R(IP1)=X0
      DO 127 J=1,M
      DO 127 IP1= 1,I1
  127 X(J)=X(J)-R(IP1)*W(J,IP1)
      RETURN
      END
      SUBROUTINE SKEPTIC(H,IH,JH,E,W,MH,LEV)
C DIMENSION ARRAYS SAME AS IN TET AND MEERA
      DIMENSION H(1275),IH(1275),JH(1275),E(4),RSQ(4),RAB(4),W(200,4)
      COMMON R(200,4)
      DO 4 L=1,4
      RSQ(L)=0.
      RAB(L)=0.
      DO 3 I=1,LEV
    3 R(I,L)=0.
      DO 1 I=1,MH
      C1=IH(I)
      C2=JH(I)
      II=IH(I)
      JJ=JH(I)
      IF(E(L).EQ.0.)E(L)=1.0E-20
      IF((C1-C2)**2.LT.0.1) GO TO 2
      R(II,L)=R(II,L)+H(I)*W(JJ,L)/E(L)
      R(JJ,L)=R(JJ,L)+H(I)*W(II,L)/E(L)
      GO TO 1
    2 R(II,L)=R(II,L)+(H(I)-E(L))*W(II,L)/E(L)
    1 CONTINUE
      DO 4 I=1,LEV
      RSQ(L)=RSQ(L)+R(I,L)**2
    4 RAB(L)=RAB(L)+ABS(R(I,L))
      DO 5 L=1,4
    5 RSQ(L)=SQRT(RSQ(L))
      PRINT 6,(RSQ(L),L=1,4)
    6 FORMAT(/* FOR THE FOUR E-VECTORS, W, THE RMS MAGNITUDES OF VECTORS
     1 R=(1/E)(H-E)W ARE*//4E20.5)
      PRINT 7,(RAB(L),L=1,4)
    7 FORMAT(/* AND THE FOUR SUMS OF ABSOLUTE VALUES OF COMPONENTS OF VE
     1CTORS, R, ARE*//4E20.5)
      PRINT 8
    8 FORMAT(/* FOR THE FOUR E-VECTORS, THE COMPONENTS R(I)   (AND THE R
     1ATIOS ABS(R(I)/W(I)) )   ARE*)
      DO 9 I=1,LEV
      DO 10 L=1,4
   10 RSQ(L)=ABS(R(I,L)/W(I,L))
      PRINT 11,(R(I,L),RSQ(L),L=1,4),I
    9 CONTINUE
   11 FORMAT (/4(E10.2,*(*,E8.2,*)*),5X,I5)
      RETURN
      END
      SUBROUTINE EZERO(LEVELS,LEV,IX,W)
      DIMENSION L(10),N(10),IX(10,200),W(200,4)
      IBOTM=1
      ITOP=2
      SIGMA=0.025
```

```
      A=90.
      L(1)=3
      L(2)=1
      L(3)=1
      L(4)=4
      N(1)=3
      N(2)=3
      N(3)=3
      N(4)=4
      RATIO=7.0278954884E-01
      R2=0.
      R4=0.
      DO 12 K=1,LEV
      DO 12 I=1,LEVELS
      PIX=IX(I,K)
      PN=N(I)
      PL=L(I)
      R2=R2+W(K,IBOTM)*W(K,ITOP)*PIX*2.*(PN+1.5)
      R4=R4+W(K,IBOTM)*W(K,ITOP)*PIX*2.*(1.5*PN*(PN+3.)-0.5*PL*(PL+1.))
   12 CONTINUE
      R2=R2*(RATIO/A**(1./3.))
      R4=R4*(RATIO**2/A**(2./3.))
      RHO2=R2**2
      RHO=(R2-SIGMA*R4)**2
      PRINT 13,R2,R4
   13 FORMAT (/41H THE MATRIX ELEMENTS OF R**2 AND R**4 ARE,2E20.10)
      PRINT 15,RHO2
   15 FORMAT (/24H WHEN SIGMA=0, RHO**2 IS,E20.10)
      PRINT 16,SIGMA,RHO
   16 FORMAT (/14H WHEN SIGMA IS,F9.4,10H RHO**2 IS,E20.10)
      RETURN
      END
```

```
      PROGRAM SLATER(INPUT,OUTPUT,PUNCH)
      COMMON BB
      DIMENSION N(10),L(10),NN(4),LL(4)
      DIMENSION S(10,10)
      IDUMMY=0
      LEVELS=5
      A=140.
      BB=1.005991*A**(1./6.)
      READ 1, (N(I),I=1,LEVELS)
      READ 1, (L(I),I=1,LEVELS)
    1 FORMAT (10I5)
      DO 10 I=1,LEVELS
      DO 10 J=1,I
      NN(1)=N(I)
      NN(2)=N(I)
      NN(3)=N(J)
      NN(4)=N(J)
      LL(1)=L(I)
      LL(2)=L(I)
      LL(3)=L(J)
      LL(4)=L(J)
      S(I,J)=RADIAL(IDUMMY,NN,LL)
      PRINT 2, (NN(K),LL(K),K=1,4),S(I,J)
   10 CONTINUE
    2 FORMAT(/4(2I5,5X),E20.10)
      DO 11 I=1,LEVELS
      PUNCH 3, (S(I,J),J=1,I)
      PRINT 4, (S(I,J),J=1,I)
   11 CONTINUE
    3 FORMAT (10F8.5)
    4 FORMAT (/10F8.5)
      STOP
      END
      FUNCTION RADIAL(K,N,L)
      COMMON BB
      DIMENSION N(4),L(4)
      DIMENSION A(4),B(4),C(4),G(2,5)
      PI=3.1415927
      DO 16 I=1,4
      R=N(I)-1
      RR=L(I)
      IF(R-0.1)10,11,11
   10 A(I)=1.
      B(I)=0.
      C(I)=0.
      GO TO 16
   11 IF(R-1.-0.1)12,13,13
   12 A(I)=SQRT(RR+3./2.)
      B(I)=-1./A(I)
      C(I)=0.
      GO TO 16
   13 IF(R-2.-0.1)14,15,15
   14 A(I)=SQRT((RR+3./2.)*(RR+5./2.)*0.5)
      B(I)=-SQRT((2.*(RR+5./2.))/(RR+3./2.))
      C(I)=0.5/A(I)
```

```
      GO TO 16
   15 PRINT1
    1 FORMAT(6H ERROR)
   16 CONTINUE
      DO 17 I=1,2
      G(I,1)=A(I)*A(I+2)
      G(I,2)=A(I)*B(I+2)+B(I)*A(I+2)
      G(I,3)=A(I)*C(I+2)+C(I)*A(I+2)+   B(I)*B(I+2)
      G(I,4)=B(I)*C(I+2)+C(I)*B(I+2)
   17 G(I,5)=C(I)*C(I+2)
      RADIAL=0.
      DO 18 I=1,5
      DO 18 J=1,5
      II=L(1)+L(3)+2*(I-1)
      JJ=L(2)+L(4)+2*(J-1)
   18 RADIAL =RADIAL+G(1,I)*G(2,J)*FFF(K,II,JJ)
      RADIAL=RADIAL*SQRT(2.**(L(1)+L(2)+L(3)+L(4))/(FFAC(2*L(1)+1)*FFAC(
     12*L(2)+1)*FFAC(2*L(3)+1)*FFAC(2*L(4)+1)))
      RADIAL=RADIAL*16./PI
      RETURN
      END
      FUNCTION FFF(K,M1,M2)
C WHEN CALLED BY RADIAL, THIS FUNCTION GIVES DELTA-FORCE RADIAL INTEGRAL
C  THE POTENTIAL STRENGTH IS 500 MEV FERMI**3
      COMMON BB
      PI=3.1415927
      SIG=(-1.)**(M1+M2)
      IF(SIG)10,10,11
   11 N=(M1+M2+2)/2
      FFF=FFAC(2*N-1)*SQRT(PI/2.)*500./(2.**(2*N+1)*4.*PI*BB**3)
      RETURN
   10 N=(M1+M2+2-1)/2
      FFF=FAC(N)*500./(2.**(N+2)*4.*PI*BB**3)
      RETURN
      END
      FUNCTION FAC(I)
      FAC=1.
      DO 1 L=1,I
      R=L
    1 FAC=FAC*R
      RETURN
      END
      FUNCTION FFAC(I)
      FFAC=1.
      K=(I+1)/2
      DO1 L=1,K
      R=2*L-1
    1 FFAC=FFAC*R
      RETURN
      END
```

```
      PROGRAM TRANONE (INPUT,OUTPUT)
      DIMENSION IX(10,200),W(200,4),IXO(10,200),WO(200,4),IO(10)
      DIMENSION Z(4,4)
      IDECKS=4
      DO 20 IDUM=1,IDECKS
C READ IN EVEN-A DATA
      READ 5, (IO(I),I=1,10)
    5 FORMAT (10I5)
      DO 32 K=1,200
      DO 40 L=1,4
   40 W(K,L)=0.
      DO 32 I=1,10
   32 IX(I,K)=0
      READ 1,LEV,LEVELS
    1 FORMAT (I5,5X,I5)
      DO 11 K=1,LEV
      READ 3,(W(K,L),L=1,4),(IX(I,K),I=1,LEVELS)
   11 CONTINUE
    3 FORMAT (4X,4E16.7,2X,10I1)
C READ IN ODD-A DATA, ONE LEVEL AT A TIME
C  SET NN TO THE NUMBER OF ODD DECKS TO BE READ IN
      NN=4
      DO 20 III=1,NN
C SET IWHAT TO 0 FOR STRIPPING, TO 1 FOR PICKUP
C SET IGO = NO. OF LEVEL IN ODD-A TO/FROM WHICH TRANSFER IS MADE
C  SET IEVEN TO NUMBER OF STATES OF EVEN NUCLEUS TO BE USED
C  SET IODD TO NUMBER OF STATES OF GIVEN J OF ODD NUCLEUS TO BE USED
      READ 5, IWHAT,IGO,IEVEN,IODD
      WHAT=IWHAT
      DO 36 K=1,200
      DO 41 L=1,4
   41 WO(K,L)=0.
      DO 36 I=1,10
   36 IXO(I,K)=0
      READ 1, LEVO,LEVELS
      DO 13 K=1,LEVO
      READ 3, (WO(K,L),L=1,4),(IXO(I,K),I=1,LEVELS)
   13 CONTINUE
      DO 31 K=1,LEV
      PRINT 30,(IX(I,K),I=1,10),(W(K,L),L=1,4),(IXO(I,K),I=1,10),(WO(K,L
     1),L=1,4)
   31 CONTINUE
   30 FORMAT (1X,10I1,4E14.5,2X,10I1,4E14.5)
      IF(WHAT-0.1)22,22,23
   22 CONTINUE
C ***************      STRIPPING    ************
C TAKE AN IXO AND COMPARE TO ALL IX-S
      DO 44 I=1,4
      DO 44 J=1,4
   44 Z(I,J)=0.
      DO 14 KO=1,LEVO
      DO 14 K=1,LEV
      ER=0.
      DO 16 I=1,LEVELS
      R=IX(I,K)-IXO(I,KO)
```

```
   16 ER=ER+R**2
C IF IT IS THE SAME, ADD WO*W*(   )  TO Z
      IF(ER-0.1) 17,17,14
   17 R=IX(IGO,K)
      RR=IO(IGO)
      R=R/RR
      IF(1.-R)14,14,34
   34 CONTINUE
      DO 45 LE=1,IEVEN
      DO 45 LO=1,IODD
   45 Z(LE,LO)=Z(LE,LO)+WO(KO,LO)*W(K,LE)*SQRT(1.-R)
   14 CONTINUE
      DO 46 LE=1,IEVEN
      DO 46 LO=1,IODD
      Z(LE,LO)=Z(LE,LO)**2
   46 PRINT 4, LE,LO,Z(LE,LO)
    4 FORMAT(/* THE SQUARED MATRIX ELEMENT OF A+ FROM LEVEL*,I5,*  OF EV
     1EN-A TARGET TO THE NUMBER*,I5,*  LEVEL OF GIVEN J IN ODD NUCLEUS I
     2S*//E40.10///)
      GO TO 20
C        ***************      PICK-UP      ****************
C TAKE AN IXO AND COMPARE TO ALL IX
   23 DO 47 I=1,4
      DO 47 J=1,4
   47 Z(I,J)=0.
      DO 24 KO=1,LEVO
      DO 24 K=1,LEV
      ER=0.
      DO 25 I=1,LEVELS
      RR=IGO-I
      IF(RR**2-0.1)26,26,27
   26 R=IX(I,K)-(IXO(I,KO)+1)
      GO TO 25
   27 R=IX(I,K)-IXO(I,KO)
   25 ER=ER+R**2
C IF IXO IS THE SAME AS IX, EXCEPT ONE LESS IN THE PICK-UP LEVEL
C  THEN ADD WO*W*(   ) TO Z
      IF(ER-0.1)28,28,24
   28 R=IX(IGO,K)
      RR=IO(IGO)
      R=R/RR
      IF(R)24,24,35
   35 CONTINUE
      DO 48 LE=1,IEVEN
      DO 48 LO=1,IODD
   48 Z(LE,LO)=Z(LE,LO)+WO(KO,LO)*W(K,LE)*SQRT(R)
   24 CONTINUE
      DO 49 LE=1,IEVEN
      DO 49 LO=1,IODD
      Z(LE,LO)=Z(LE,LO)**2
   49 PRINT 6,LE,LO,Z(LE,LO)
    6 FORMAT(/* THE SQUARED MATRIX ELEMENT OF A- FROM LEVEL*,I5,*  OF EV
     1EN-A TARGET TO THE NUMBER*,I5,*  LEVEL OF GIVEN J IN ODD NUCLEUS I
     2S*//E40.10///)
   20 CONTINUE
      STOP
      END
```

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