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Playing with the Collective State

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We examined the condition for a large energy-shift of a single unperturbed level, due to the residual interaction, in a nuclear many-body system. No separability assumption as made in the schematic model has been considered. A simple algorithm for calculating the energy of the corresponding state is presented.

Examina-se a condição para que haja um deslocamento grande de um único nível não perturbado, pela presença da interação residual, em um sistema nuclear de muitos corpos. Não se faz hipótese alguma de separa' bilidade, ao contrário do que ocorre no modelo esquemãtico. E apresenta-se um algoritmo bastante simples para se calcular esse deslocamento de energia.

1. INTRODUCTION

The treatment of the nuclear many body problem is based on the independent particle approximation, i.e. the shell model. The model Hamiltonian

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H, describes independent: particle degrees of freedom and the levels of its energy spectrum occur in well separated bunches which is characteristic of the shell model. It is observed experimentally that the energy spectrum of a many-body system usually contains one or more levels of collective character. The total Hamiltonian of the many-body system is given by the model Hamiltonian H plus a residual two body interaction V, and the collective levels would result from a strong mixture of levels in a bunch, caused by this residual interaction. In ideal cases, the resulting energies are strongly shifted with respect to the center of the bunch of unperturbed energies.

Physically, the collective states are explained in terms of particle--hole excitations and the schematic model as described in Ref.1 supplies some mathematical insight for that large energy shift. The schematic model is based on the separability assumption of the matrix elements of V in the model space. However, such separability is not valid in general so we eliminate here this restriction and discuss necessary and sufficient conditions for the residual interaction to shift one of the energy levels of a bunch of unperturbed energy levels.

Starting from the eigenvalue problem in the form of a secular determinant, we exhibit in Section 2 the condition for occuring a strong energy shift in a <u>single</u> level. This leads at the same time to a simple algorithm for calculating this energy shift. As an illustration we give in Section 3 results of âalculations performed with this algorithm using schematic and realistic Warniltonians.

2. CONDITION FOR A LARGE ENERGY SHIFT, OR WHEN DOES A STRONG ENERGY SHIFT ARISE?

We are interested in physical many body systems for which it is appropriate to cast the energy eigenvalue problem into the form

$$\sum_{j} (H_{ij} - E\delta_{ij})c_j = 0 , \qquad (2.1)$$

where $c_j = \langle \Phi_j | \Psi \rangle$ are the components of the many body wave function Ψ in a suitable model space spanned by a subset of eigenstates $\{\Phi_j\}$ of H

(the many body unperturbed Hamiltonian), and H_{ij} is given in terms of the unperturbed energies E, and the residual interaction V by

$$H_{ij} = E_i \delta_{ij} + \langle \Phi_i | V | \Phi_j \rangle .$$

We introduce the average energy E^0 of a bunch of N unperturbed energies,

$$E^{0} = \frac{1}{N} \sum_{i=1}^{N} E_{i}$$
,

and the energy shifts will be measured from it. Let us then find the conditions under which a <u>single</u> energy eigenvalue E, in (2.1), is strongly shifted (either up or down) by 'V with respect to E^0 .

With $\varepsilon = E - E^0$ and $\varepsilon_i = E_i - E^0$, the eigenvalue problem (2.1) reads

$$|\varepsilon_i \ 6_{ij} + V_{ij} - \varepsilon \ \delta_{ij}| \equiv |h_{ij} - \varepsilon \ \delta_{ij}| = 0.$$

For large $|\varepsilon|$, we may extract from each line the factor e and the resulting determinant

$$\sum_{P(i_1i_2...i_N)} (-)^{P(\frac{h_{1i_1}}{\epsilon} - \delta_{1i_1})(\frac{h_{2i_2}}{\epsilon} - \delta_{2i_2})....(\frac{h_{Ni_N}}{\epsilon} - \delta_{Ni_N}) = 0$$

(the sum is over all possible permutations, P, of i_1 , i_1 , \dots i_n) is then expanded in powers of (h/ε) :

$$1 + \frac{\alpha_1}{\varepsilon} + \frac{\alpha_2}{\varepsilon^2} + \ldots + \frac{\alpha_N}{\varepsilon^N} = 0 \quad . \tag{2.2}$$

Here

$$\alpha_{k} = (-)^{k} \sum_{i_{1} > i_{2} > \dots > i_{k}} d_{i_{1}i_{2}} \cdots i_{k}, \qquad (2.3)$$

where $d_{i,i}$ are the determinants corresponding to the submatrices of h_{ij}^{1} containing rows and columns i_{12} ... i_k . Specifically,

$$a_{1} = -\operatorname{Tr} h = -\sum_{i} h_{ii}$$

and

$$\alpha_N = (-)^N |h_{ij}|$$

Due to trace invariance, the trace of h is also given by the sum of the N eigenvalues of Eq.(2.2). Thus $(-\alpha_1)$ is the maximum possible energy shift and occurs if $\alpha_k \equiv 0$ for $k \geq 2$. It is clearly sufficient that α_k / ε^k be small for k > 1 in order to have a single strongly shifted level. This condition will be fulfilled if the nondiagonal matrix elements are comparable in magnitude to the diagonal ones, as can be seen for instance from the expression

$$\alpha_{2} = \sum_{i>j} (h_{ii}h_{jj} - h_{ij}h_{ji})$$

Thus if α_k / ϵ^k is small for k > 1, the strong correlations we need between the states can be built up.

We now show that the relative smallness of higher order terms in (2.2) is also **a** necessary condition for the occurrence of a strong energy shift. Indeed, let e, e_2 , $\dots e_N$ be the roots of (2.2). Then,

$$\alpha_{1} = -\sum_{i=1}^{N} e_{i} \qquad (2.4a)$$

$$\alpha_2 = \sum_{i < j} e_i e_j \qquad (2.4b)$$

$$\alpha_{3} = -\sum_{i < j < k} e_{i} e_{j} e_{k} \qquad (2.4c)$$

$$\alpha_N = (-)^N e_1 e_2 \dots e_N$$
 (2.4d)

Assuming that $|e_1| >> |e_k|$, for k > 1, the order of magnitude of the terms of Eq.(2.2) for this root e_1 are roughly

$$\frac{\alpha}{\varepsilon_1} = \mathcal{O}(1) , \quad \frac{\alpha}{\varepsilon_1^2} = \mathcal{O}(\Sigma \quad \frac{\varepsilon_1}{\varepsilon_1}), \quad \dots \quad .$$

Thus the higher order terms are small when there is a single strongly shifted energy level.

Remark: If two energy eigenvalues were strongly shifted then clearly α_2/ϵ^2 would be comparable in magnitude to the first two terms in (2.2) as is obvious from expressions (2.4a,b).

The eigenvalue problem in form (2) will now be solved for the largest ei-genvalue, using the following simple linearised scheme. We consider Eq. (2.2) truncated after the k^{th} term. In order to solve it for the largest eigenvalue, we put

$$1 + \frac{\alpha_1}{\varepsilon} \approx 0 \tag{2.5a}$$

$$1 + \frac{\alpha_1}{\varepsilon^{(2)}} + \frac{\alpha_2}{\varepsilon^{(2)}\varepsilon^{(1)}} = 0$$
(2.5b)

$$\frac{1}{\epsilon} + \frac{\alpha_1}{\epsilon^{(k)}} + \frac{\alpha_2}{\epsilon^{(k)}\epsilon^{(k-1)}} + \dots + \frac{\alpha_k}{\epsilon^{(k)}\epsilon^{(k-1)}\dots\epsilon^{(1)}} = 0$$
 (2.5c)

and

$$1 + \frac{\alpha_1}{\varepsilon(n)} + \frac{\alpha}{\varepsilon(n)\varepsilon}(n-1) + \cdots + \frac{\alpha_k}{\varepsilon(n)\varepsilon(n-1)\cdots\varepsilon(n-k+1)} = 0, \text{ for } n > k.$$
(2.5d)

Equations (2.5a-c) determined the starting values for the iteration scheme (2.5d). In case of convergence, $\lim_{n \to \infty} 1/\epsilon^{(n)} \equiv 1/\epsilon_k$ obviously solves the

truncated equation. The convergence of ε_k towards the desired eigenvalue is very fast if the higher order correction terms are small. This can be seen from the numerical examples given in Section 3.

Let us look into the conditions for convergence of the iteration scheme (2.5d), starting with k = 2:

$$1 + \frac{\alpha_1}{\epsilon^{(n)}} + \frac{\alpha_2}{\epsilon^{(n)}\epsilon^{(n-1)}} = 0$$
 (2.6a)

or

$$\frac{1}{\varepsilon^{(n)}} = \frac{-1}{\alpha_1 + \frac{\alpha_2}{\varepsilon^{(n-1)}}}$$
(2.6b)

This recurrence relation generates a continued fraction expansion for which the initial value is given by (2.5a):

$$\frac{1}{\varepsilon^{(1)}} = -\frac{1}{\alpha_1}$$

•

It is proved in the Appendix that the limit of $1/\epsilon^{(n)}$ for $n \to \infty$ exists only if $a_1^2 \ge 4\alpha_2$. The limit value is given by the root of Eq. (2.6a) with the largest magnitude.

The iteration scheme for k > 2 has the same form (2.6b):

$$\frac{1}{\varepsilon} = \frac{-1}{\alpha_1 + \frac{\tilde{\alpha}_2}{\varepsilon(n-1)}}, \qquad (2.6c)$$

•

with an effective $\tilde{\alpha}_{2}$ which, for k = 3, is given by

$$\tilde{\alpha}_2 = \alpha_2 + \frac{\alpha_3}{\varepsilon^{(n-2)}}$$

The condition for convergence is now $\alpha_1^2 \ge 4 \tilde{\alpha}_2$ (the condition should be $\alpha_1^2 \ge \tilde{\alpha}_2$ where $\tilde{\alpha}_2$ is the limit for $n \to \infty$ of $\tilde{\alpha}_2$ but we shall assume that

 $\tilde{\alpha}$ is stabilised). One sees that the smaller the higher order terms, the larger the energy shift of the resulting eigenvalue E.

It is amusing to note that the a's can be obtained by the following graphical prescription. The states Φ_i are represented by a line (labeled i), the operator h by a "cross" x (like a one body operator), and h_{ij} is drawn as

$$h_{ij} = \sum_{i=1}^{j} \cdots \times k_{i}$$

using the convention that the first label corresponds to the lineleaving the **vertex and** the second to the line arriving at **it**. We exhibit **in** Fig. 1 the diagramatic expressions for a few of the α_{i} 's.



The rules for calculating the diagrams are the usual ones: each closed loop carries a minus sign and one has to sum over all permutations of the labels. The 5th graph of α_{μ} , for instance, confains 4! = 24 terms corresponding to the determinantal expression (2.3).

Finally, let us consider the expansion coefficients $c_{\chi} = \langle \Phi_{\chi} | \Psi \rangle$ of Eq. (2.1). Putting $c_N = 1$, they are given as

$$c_{k} = \frac{\left| \begin{pmatrix} h_{ij} - \epsilon \ \delta_{ij} \end{pmatrix} \overline{\delta}_{jk} - \delta_{jk} \ h_{iN} \right|}{\left| h_{ij} - \epsilon \ \delta_{ij} \right|}, \ k = 1, 2, \dots, N-1,$$

where $\overline{\delta}_{jk} \equiv 1 - \delta_{jk}$, both determinants being (N-1) dimensional. Expanding again in powers of h/ϵ , we have

$$e_{k} = -\frac{\frac{1}{\varepsilon} d^{(k)} - \frac{1}{\varepsilon^{2}} \sum_{i}^{\varepsilon} d^{(k)}_{i} + \frac{1}{\varepsilon^{3}} \sum_{i < j}^{\varepsilon} d^{(k)}_{ij} + \dots}{1 + \frac{\alpha'_{1}}{\varepsilon} + \frac{\alpha'_{2}}{\varepsilon^{2}} + \dots}$$

where $\alpha_k^{\mathbf{j}}$ are the expressions (2.3) restricted to the (N-1) dimensional submatrices of h_{ij} and $d_{ij}^{(k)}$ are the subdeterminants built out of the rows ij... and k, and columns ij... and N.

Thus, for instance

$$d^{(k)} \equiv -h_{kN}$$
 , (2.7a)

$$d_{i}^{(k)} \equiv \begin{vmatrix} h_{ii} - h_{iN} \\ h_{ki} - h_{kN} \end{vmatrix} , \qquad (2.7b)$$

$$d_{ij}^{(k)} \equiv \begin{vmatrix} h_{ii} & h_{ij} - h_{iN} \\ h_{ji} & h_{jj} - h_{jN} \\ h_{ki} & h_{kj} - h_{kN} \end{vmatrix}$$
(2.7c)

We consider the lowest order approximation for $c_{\not\!k}$ by inserting into its expression

$$\varepsilon^{(1)} = \sum_{i=1}^{N} h_{ii}.$$

Using (2.7a), we can write

$$e_{k}^{(1)} = \frac{h_{kN}}{\varepsilon^{(1)} - \sum_{i=1}^{N-1} h_{ii}} = \frac{h_{kN}}{h_{NN}} .$$

The transition amplitude induced by an operator 0 from that state described by ci') to another state $|X\rangle$ is proportional to

$$\sum_{k} \langle X | 0 | \Phi \rangle \langle \Phi_{k} | h | \Phi_{N} \rangle ,$$

which is a coherent sum and thus strongly enhanced for operators which have the same signature in their matrix elements as the Hamiltonian h. Example in the schematic model is the multipole operator used for 0 and h.

3. NUMERICAL EXAMPLES

Let us first consider a few simple examples. The ideal cases for a maximal shift (up or down) of a single energy eigenvalue are those of Hamiltonians with constant matrix elements:

$$(h_{ij}) = \begin{pmatrix} A & A & \cdots \\ A & A & \cdots \\ \vdots & \vdots & \vdots \\ \vdots & \ddots & \vdots \\ \vdots & \ddots & \vdots \end{pmatrix}$$

In this case, clearly all the subdeterminants of order $k \ge 1$ are zero. Thus, there is only one eigenvalue different from zero, $\varepsilon = NA$, N being the dimension of the matrix, the other (N-1) eigenvalues being zero.

In order to see how the iteration scheme (2.5d) does work, we consider next the less trivial matrix

In Table 1, we exhibit for N=10 the first few relevant α_k 's, the convergent energies ε_k of the continued fraction expansions and the effective $\tilde{\alpha}_2$, entering into these expansions.

Table 1

k	a k	е k	ã
1	-10.00	10.00	-
2	8.55	9.06	8.55
3	- 3.36	9.10	8.18
4	0.78	9.10	8.19

Clearly, the condition $\alpha_1^2 \ge 4 \ \tilde{\alpha}_2$ is satisfied and the convergence of the ε_k 's to the exact eigenvalue E = 9.10 is quite fast. The exact eigenvalues are obtained by diagonalisation of the matrix (2.8) which gives rise to one eigenvalue equal to 9.10, all the others being degenerate and equal to 0.1.

As a **less** favorable case, we consider a matrix whose diagonal matrix elements equal twice the off diagonal ones:

The corresponding numbers are given in Table 2.

The condition $\alpha_1^2 \ge 4 \ \tilde{\alpha}_2$ is again satisfied but the exact eigenvalue E = 5.5 is reached only by taking higher orders into account. It is clearly possible to redefine de zero of the energy thereby reducing the difference between diagonal and nondiagonal elements and then the iteration scheme will again converge very fast. Note that for these simple cases, (2.8) and (2.9), it is possible to solve the problem immediately by subtracting from the diaganal matrix elements 0.1 and 0.5, respectively, as these subtractions will produce constant matrices whose solutions are obtained trivially (1st example presented) and, in order to obtain the ac-

Table 2	2
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k	ak	ε _k	ã 2
1	-10.00	10.00	-
2	33.75	divergent	23.75
3	-60.00	6.06	23.87
4	65.63	5.38	24.88

tual eigenvalues, one has simply to add to these solutions the amount which has been subtracted from the original diagonal matrix elements.

As a further illustration, we take a realistic case, using as residual interaction (i) δ = force and (ii) Sussex matrix elements⁴.

2⁺ state at 4.43 MeV in ¹²C

(i) This calculation was done in Ref.2 assuming that this state can be described by a superposition of seven particle-hole states as given in Table 3; the unperturbed energies E_{i} taken from experiment².

Table 3

Configur hole	ation , particle	E:(MeV)
ls 1/2	1 <i>d</i> _{3/2}	33.63
ls _{1/2}	1d _{5/2}	29.80
1p3/2	² <i>p</i> _{1/2}	29.84
1p _{3/2}	² p _{3/2}	27.64
1p _{3/2}	1f _{5/2}	32.14
1p _{3/2}	¹ f _{7/2}	25.74
1p _{3/2}	¹ <i>p</i> _{1/2}	13.77

The two-body interaction used² is a simple 8-force which results in the following particle-hole matrix elements

$$V_{ij} = J_{ij} (-a_i a_j + b_i b_j) , \qquad (2.10)$$

where the a's and b's are simple geometrical expressions (see Eqs. (2. 3a) and (2.3b) of Ref.2) and J_{ij} are the radial matrix elements given in Table 2 of the same reference. If one had assumed constant radial matrix elements, the interaction would be separable. The average energy with respect to which the shift is calculated is $E^0 = 27.509$ MeV. The results for the iteration scheme are presented in Table 4.

Table 4

k	a k	ε k	ã
1	18.55	-18.55	-
2	-161.0	-24.99	-161.0
3	-1054	-23.49	-116.1
4	6342	-23.04	-103.4

The exact result, obtained by diagonalization of the matrix, is -23.08 MeV. Adding E^0 to the resulting ε_k , one obtains E = 4.39 MeV (the strength of the δ -force has been adjusted to reproduce this 2⁺ state).

(ii) Same as in (i) using the $Sussex^4$ matrix elements as particle - particle interaction. We used b = 1.6 fm for the harmonic oscillator size parameter. The results are shown in Table 5.

k	α_k	ϵ_k	ã ₂	
1	1.90	-1.90	-	
2	-167.8	-12.80	-167.8	
3	649.1	-15.46	-209.8	
4	1613	-15.25	-203.4	

Table 5

Adding E^0 to the resulting ε_{ν} , one obtains E = 12.26 MeV.

For both cases (i) and (ii), the condition $\alpha_1^2 \ge 4 \tilde{\alpha}_2$ is satisfied and the convergence is quite fast.

4. SUMMARY

We have shown that in order to determine the energy ε of a state which is strongly shifted, with respect to its unperturbed position, by a residual force, it is simply necessary to calculate the sum of the subdeterminants of the full Hamiltonian matrix. These sums α_k enter into low order equations for ε which allow in addition for a simple recursive solution in form of a continued fraction expansion. The smallness of α_k/ε^k for k > 1, is a necessary and sufficient condition for the occurrence of a large shift. In view of the simplicity of that procedure, compared to the full N-dimensional problem, we have the feeling that there should be a corresponding simplification in a microscopic many-body calculation of such a collective state.

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APPENDIX

The continued fraction expansion (2.5b) or, in general, (2.5c) (assuming a stabilised $\tilde{\alpha}_{2}$) is generated by the linear rational transformation

$$S = S(\omega) = \frac{-1}{\alpha_1 + \tilde{\alpha}_2 \omega}$$
 (A.1)

The n^{th} order approximation is then given by

$$s^{n}(\omega) \equiv s(s(s...s(\omega))...) , \qquad (A.2)$$

with $\omega = 1/\epsilon^{(1)}$. In order to establish the conditions for the existence of $\lim S^n(\omega)$, we follow Wall³. The mapping (A.1) has two fixed points

$$X_{1,2} = \frac{-\alpha_1 \pm \sqrt{\alpha^2 - 4\tilde{\alpha}}}{2\tilde{\alpha}_2} ,$$

and allows the following relations to be valid

$$S = X + X_1 \omega - X_1$$

$$S = X_2 + X_2 \omega - X_2$$
, for $\frac{X_1 \neq X_2}{1 \neq X_2}$

and

$$\frac{1}{S - \chi} = \frac{1}{\omega - X_1} - \frac{1}{X_1}, \text{ for } X_1 = X_2.$$

Therefore, the n^{th} order mapping, (A.2), obeys

$$\frac{S^{n}(\omega) - X_{1}}{S^{n}(\omega) - X_{2}} = \left(\frac{X_{1}}{X_{2}}\right)^{n} \frac{\omega - X_{1}}{\omega - X_{2}}, \text{ for } X_{1} \neq X_{2}$$
(A.3)

and

$$\frac{1}{S^{n}(\omega)} - \frac{1}{X_{1}} \quad \omega - \frac{1}{X_{1}} \quad x_{1} \quad \text{for } X_{1} = X_{2}^{-}.$$

From (A.3), it is obvious that for $n \to \infty$, the $\lim_{n \to \infty} S^n(\omega)$ has to be equal to X_1 . Thus, for $X_1 = X_1$ the continued fraction expansion converges towards X_1 . For $X_1 # X_2$ and $|X_1| < |X_2|$, we have for sufficiently large n,

$$S^{n}(\omega) - X_{1} = \delta_{n}(S^{n}(\omega) - X_{2}) ,$$

with

$$|\delta_n| = \text{const} \left| \frac{X_1}{X_2} \right| < <1$$
.

So

$$s^{n}(\omega) = \frac{x_{1} - \delta_{n} x_{2}}{1 - \delta_{n}}$$
 (A. 4)

Thus again the continued fraction expansion converges and $\lim S^n(\omega) = X_1$, which is the fixed point of smallest magnitude (largest energy).

Finally, if $|X_1| = |X_2|$ and $X \neq X_2$, the limit of the right-hand side of (A.4) obviously does not exist. Thus, the condition for convergence of (2.5b,c) is

 $\alpha_1^2 \ge 4 \alpha_2 \qquad (\alpha_1 \neq 0)$

 $\alpha_1^2 \ge 4 \tilde{\alpha}_2$

or

(assuming $\tilde{\alpha}$ estabilised).

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