CONVERGENCE OF THE LINKED GRAPH EXPANSION FOR THE GROUND STATE ENERGY OF ^{40}Ca IN A MODEL SPACE*

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The convergence of the linked graph expansion for the binding energy of ^{40}Ca is discussed in the $2\hbar\omega$ model space. It is found that when the lowest energy of the $2\hbar\omega$ states matrix is above the closed shell energy the expansion can be always made convergent. Under this condition, the first few terms of the expansion can be used to approximate the full result even if the expansion is not convergent.

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1. Introduction

The properties of the perturbation expansions in the nuclear shell model have received much attention in recent years. The pioneering calculations of the nuclear energy levels by Kuo and Brown [1] and by Barret and Kirson [2] have been followed by formal investigations of the convergence properties [3, 4]. In particular the role of the intruder states has been pointed out [3] and different methods of removing divergences have been suggested [4–6]. Most recently, the convergence of the Brillouin–Wigner expansion has been studied [7] and a shift of the unperturbed spectrum has been shown to improve the convergence of the expansion.

Recently the convergence of the linked graph expansion for the energy [8] and the radius [9] of ground state of ^{40}Ca has been investigated numerically in a model space of 0–$2\hbar\omega$ excitations. Using the inversion technique analogous to the Q box approach of Ref. [4], it was possible to obtain a closed sum of the expansion, which in turn has been compared with the first few terms of the expansion.

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The existence of the closed sum allows us to give a rigorous discussion of the convergence in this model case. In Section 2 we derive conditions for the convergence in terms of the lowest eigenvalue of the $2\hbar\omega$ energy submatrix and of the shift of the unperturbed spectrum. When the expansion is convergent its sum is equal to the closed sum. Next we derive limits for the exact energy in terms of the first few terms of the expansion, which are valid even when the expansion diverges. The discussion is given in Section 3.

2. *Derivation of the conditions for convergence*

The linked graph expansion in the space of the $2\hbar\omega$ excitations of Ref. [8]

$$\Delta E = \frac{H^{02}H^{20}}{a} + \frac{H^{02}V^{22}H^{20}}{a^2} + \frac{H^{02}V^{22}V^{22}H^{20}}{a^3} + \dots$$

has the closed sum

$$\Delta E = -H^{02}(H^{22})^{-1}H^{20}, \tag{1}$$

where H^{ij} are submatrices of the energy matrix

$$H = \begin{pmatrix} H^{00} & H^{02} \\ H^{20} & H^{22} \end{pmatrix}. \tag{2}$$

The superscript ^{0} denotes the closed shell state and the superscript ^{2} stands for the group of states (175 in ^{40}Ca) with $2\hbar\omega$ excitations. We have

$$H^{00} = 0, \quad H^{02} = V^{02}, \quad H^{20} = V^{20}, \quad H^{22} = V^{22}-a, \quad a = -2\hbar\omega, \tag{3}$$

where the closed shell energy H^{00} is assumed zero. The linked graph expansion is obtained by expanding ΔE of Eq. (1) in the powers of $(1/a)$. Equation (1) is further discussed in the appendix.

We shall now derive conditions for the convergence of the expansion in terms of the eigenvalues of the submatrix H^{22}. We have

$$H^{22}v^k = (V^{22}-a)v^k = (\lambda^k - a)v^k, \quad k = 1, 2 \dots 175 \tag{4}$$

where v^k are eigenvectors of H^{22} and $\eta^k = \lambda^k - a$ are the corresponding eigenvalues. The λ^k's are the eigenvalues of V^{22}. We have then for ΔE of Eq. (1)

$$\Delta E = \sum_k \frac{(d^k)^2}{a-\lambda^k}, \tag{5}$$

where

$$d^k = H^{20} \cdot v^k. \tag{6}$$

Expanding in $(1/a)$ we obtain the linked graph expansion

$$\Delta E = \sum_{r=2}^{\infty} \Delta E_r, \quad \Delta E_r = \frac{1}{a} \sum (d^k)^2 \left(\frac{\lambda^k}{a}\right)^{r-2} \tag{7}$$

with ΔE_r being of order r in the potential V.

The necessary and sufficient conditions for the convergence of the series in Eq. (7) are

$$|\lambda^k| < |a| \text{ for all } k, \text{ or } |\lambda_{\min}| < |a| \text{ and } |\lambda_{\max}| < |a|. \tag{8}$$

We assume that $d^k_{\min}$ and $d^k_{\max}$ are different from zero.

As discussed in Refs. [7, 8] and [10], the convergence can be improved by subtracting a constant s (λ_{nl} in notation of Ref. [8]) from a and from V^{22}. With this shift Eqs. (7) will become

$$\Delta E = \sum_{r=2}^{\infty} E^s_r, \quad \Delta E^s_r = \frac{1}{a-s} \sum_k (d^k)^2 \left(\frac{\lambda^k - s}{a-s}\right)^{r-2}. \tag{7a}$$

The conditions of convergence are now

$$|s-\lambda_{\min}| < |s-a| \quad \text{and} \quad |s-\lambda_{\max}| < |s-a|. \tag{8a}$$

There is no solution to Eqs. (8a) if

$$\lambda_{\min} < a < \lambda_{\max}. \tag{9}$$

If

$$\lambda_{\min} > a \tag{10}$$

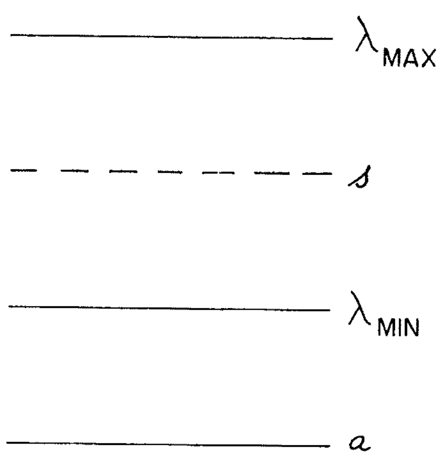

Fig. 1

one can see from Fig. 1 that conditions (8a) are equivalent to

$$s > \frac{\lambda_{\max} + a}{2}, \tag{11}$$

$$s > \frac{\lambda_{\min} + a}{2}. \tag{12}$$

Only condition (11) needs to be used because (12) follows from (11). Condition (10) can be written as

$$\lambda_{\min} - a = \eta_{\min} > 0 = H_{00} = \text{closed shell energy}, \tag{10a}$$

which says that the eigenvalues of the energy submatrix H^{22} must be greater than the closed shell energy. Under this condition, one can always find such an s (according to Eq. (11)) that the shifted linked graph expansion of Eq. (7a) will converge.

Next we shall derive limits on ΔE in terms of the first few terms of the expansion. Consider the partial sum from Eq. (7a)

$$\Delta S_n = \sum_{r=2}^{n} \Delta E_r^s, \qquad n \geqslant 2.$$

Using the identity

$$\frac{1}{1-x} - \sum_{r=2}^{n-1} x^{r-2} = \frac{x^{n-2}}{1-x}$$

we obtain for ΔE of Eq. (5)

$$\Delta E - \Delta S_{n-1} = \sum_k \frac{(d^k)^2}{a-s} \left(\frac{\lambda^k - s}{a-s}\right)^{n-2} \frac{a-s}{a-\lambda^k}.$$

When $a < \lambda_{\min}$ and n is even all terms in the sum are negative and

$$|\Delta E - \Delta S_{n-1}| \leqslant C^s |\Delta E_n^s|, \tag{13}$$

where

$$C^s = \operatorname*{Max}_k \left|\frac{a-s}{a-\lambda^k}\right| = \left|\frac{2\hbar\omega + s}{2\hbar\omega + \lambda_{\min}}\right|.$$

Equation (13) has been derived assuming $a < \lambda_{\min}$ for all even $n \geqslant 4$. Under the additional assumption $s > a$ one can extend Eq. (13) to the case of $n = 2$

$$0 > \Delta E > C^s \Delta E_2^s. \tag{14}$$

The proof of Eq. (14) is easily obtained by direct substitution of ΔE, ΔE_2^s and C^s from Eqs. (5), (7a) and (13) into Eq. (14).

3. *Discussion*

Our main result about the convergence of the expansion is condition (10) which can be written as

$$\lambda_{\min} - a = \eta_{\min} > 0 = H_{00} = \text{closed shell energy}, \tag{10a}$$

which says that the eigenvalues of the energy submatrix H^{22} must be greater than the closed shell energy. Under this condition, one can always find such an s (according to Eq. (11)) that the shifted linked graph expansion of Eq. (7a) will converge.

Condition (10a) is quite similar to one obtained by Schucan and Weidenmüller [3] which is often stated as the condition about the intruder states. The difference from (10a) is that in Ref. [3] the inequality is between the eigenvalues of the full energy matrix H and not between the eigenvalues of the submatrices. We think that the difference arises because we truncate the expansion to the $2\hbar\omega$ states. Otherwise ours is the special case, with only one state in model space, of the more general situation considered in Ref. [3].

TABLE I

Some terms and sums of the linked graph expansion from Ref. [8] in MeV

$\hbar\omega = 10.41$ MeV $G_c \neq 0$	Linked graphs					Partial sum to $r = 6$	Sum Eq. (1) ΔE
	ΔE_2	ΔE_3	ΔE_4	ΔE_5	ΔE_6		
$s = 0$	-21.90	2.00	-5.45	3.33	-3.82	-25.84	-24.07
$s = \hbar\omega$	-14.60	-3.98	-2.64	-1.20	-0.75	-23.17	

As an example we apply conditions (8), (10) and (11) to the case considered in Ref. [8]. The case we consider is one with $a = -2\hbar\omega = -20.83$ ($b = 2$ fm) and $G_c \neq 0$. The linked graph contributions for $s = 0$ and $s = \hbar\omega$ are given in Table I. We compute the eigenvalues of V^{22}

$$\lambda_{\min} = -7.35 \text{ MeV} \quad \text{and} \quad \lambda_{\max} = 27.3 \text{ MeV}.$$

According to condition (8) the expansion will not converge in the $s = 0$ case. However, for $s = \hbar\omega = 10.41$ MeV conditions (10) and (11) are satisfied and the expansion will converge. We have proved thus the conclusions of Ref. [8], which were obtained from the inspection of the first six orders of the expansion and of the expansion sum.

The even terms in Eq. (7) or (7a) are coherent sums of negative contributions and should be negative and on average larger than the odd terms, as can be observed in Table I.

We observe in Table I that the second order term alone is a good approximation to ΔE in the case when the expansion does not converge ($s = 0$). The possibility that the first few terms of a diverging linked graph expansion can give a good approximation to the full answer has been considered by Schucan and Weidenmüller [3] for a more general model problem. They concluded that this is not very likely to be correct. In our model case we proved Eqs. (13) and (14) which show that the first few terms of the expansion can be used to approximate the full result even if the expansion diverges. As an example we apply Eq. (13) to the first six terms of the diverging expansion in Table I ($s = 0$ and $n = 6$) to obtain $\Delta E \approx -22 \pm 6$ MeV in agreement with $\Delta E = -24.07$ MeV.

Thus our result seems to provide a justification for adjusting parameters in a formalism so as to suppress the last computed order of the perturbation expansion, even if the terms in the following orders become large again. Eq. (14) which uses only ΔE_2^s provides a weaker limit. For $s = 0$ we obtain $\Delta E \gtrsim -34$ MeV.

The sum (1) for ΔE derives its physical meaning from the convergence of the linked graph expansion. One could ask if ΔE could be obtained from Eq. (1) or Eq. (5) when the condition (10a) is not true and the linked graph expansion does not converge. We suggest that this is not possible. When $\lambda_{\min} < a$ sum ΔE in Eq. (5) is very sensitive to small changes in eigenvalues λ^k which are near to a and consequently it is very unstable with respect to small changes in the potential V.

Similar considerations apply to the convergence of the linked graph expansion of $r_{\rm rms}^2$. The sum of the linked graph expansion truncated to $2\hbar\omega$ space is [9].

$$\Delta r^2 = 2R^{02}(H^{22})^{-1}V^{20} + (2b^2/A)V^{02}(H^{22})^{-2}V^{20}, \tag{15}$$

where R^{02} has as components the matrix elements of r^2 between the closed shell state and the $2\hbar\omega$ states, b is the oscillator constant and A is the number of nucleons. Only H^{22} depends on a and therefore the conditions of convergence for Δr^2 are the same as for ΔE. The first term in Eq. (15) will converge faster than the second term. For $b = 2$ fm $\Delta r^2 = -2.03\ \text{fm}^2$ as compared with $r_{00}^2 = 12\ \text{fm}^2$.

APPENDIX

That expression (1) is indeed the linked graph expansion in the space of $2\hbar\omega$ excitations may be shown as follows:

The linked graph expansion illustrated for a closed shell system in Fig. 2 can be written as

$$\Delta E = \frac{H^{02}H^{20}}{a} + \frac{H^{02}V^{22}H^{20}}{a^2} + \frac{H^{02}V^{22}V^{22}H^{20}}{a^3}, \ldots \tag{A1}$$

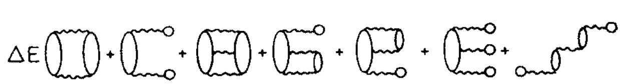

Fig. 2. Closed shell linked graph expansion for the ground state energy including all $2\hbar\omega$ excitations (all exchange and topologically equivalent graphs implied)

since in this space expression (A1) involves no unlinked graphs. Define

$$G^{22} \equiv \frac{1}{a}(H^{22} + V^{22}G^{22})$$

$$= \frac{1}{a}\left(H^{22} + \frac{V^{22}}{a} + \frac{V^{22}V^{22}}{a^2} + \frac{V^{22}V^{22}V^{22}}{a^3} + \ldots\right). \tag{A2}$$

In terms of G^{22}

$$\Delta E = H^{02}G^{22}H^{20}, \tag{A3}$$

but from Eq. (A2)

$$\left(U^{22}-\frac{V^{22}}{a}\right)G^{22}=\frac{U^{22}}{a}$$

implying

$$G^{22}=\frac{U^{22}}{a\left(U^{22}-\dfrac{V^{22}}{a}\right)}=\frac{U^{22}}{H^{22}}\,. \tag{A4}$$

Substitution of expression (A4) into (A3) yields expression (1).

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