Comment on “No core calculations” of the spectra of light nuclei

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Abstract

We comment upon a recent work of Zheng et al. concerning calculations of spectra of light nuclei with no core, where an effective interaction is constructed which spans over several shells. It is demonstrated that the omission of the particle-particle ladder diagrams in their calculations, explains the large differences between results obtained with various model spaces. We use this to infer that low-order perturbation theory works well in reproducing the binding energy of the system we consider.

PACS number: 21.60.Cs
I. INTRODUCTION

Recently, Zheng et al. [1] (hereafter ZBJVM) have presented an approach meant to circumvent the notorious intruder state problem. Moreover, this approach was devised in order to avoid calculations of complicated Feynman-Goldstone diagrams which arise in perturbation theory. It is a well-known fact that the presence of so-called intruder states may lead to the divergence of the order-by-order perturbative expansion for the effective interaction $H_{\text{eff}}$. The latter is understood to be evaluated from perturbative many-body techniques and is defined within a physically selected model space, which is given by a projection operator $P$. The remaining degrees of freedom are accounted for by the perturbative expansion. These degrees of freedom are represented by a projection operator $Q$, so that $P + Q = 1$ and $PQ = 0$. The idea behind the work of ZBJVM is, through the use of an enlarged model space, to avoid both the intruder state problem and that of calculating many perturbative contributions.

In this comment we show that the effective interactions derived by Zheng et al. may not be consistent with the underlying theory for the effective interaction. Our points are discussed in the next three sections. In Section II we discuss the omission of particle-particle ladders diagrams in the calculations of ZBJVM. Section III critically discusses the use of the starting energy as a variable. In Section IV a brief discussion of the non-hermiticity of the effective interaction is also included, and our conclusions are drawn in Section V.

II. NO-CORE SHELL-MODEL CALCULATIONS WITH THE $G$-MATRIX

The first step in the calculations of Ref. [1] is to evaluate the nuclear reaction matrix $G$ given by

$$G = V + V \frac{Q}{\omega - H_0} G,$$  \hspace{1cm} (1)

where $\omega$ is the unperturbed energy of the interacting nucleons, and $H_0$ is the unperturbed hamiltonian. The operator $Q$, commonly referred to as the Pauli operator, is a projection
operator which prevents the interacting nucleons from scattering into states occupied by other nucleons. There are many ways to handle the Pauli operator of Eq. (1). Two of these are demonstrated in Fig. 1. In (a) we show the Pauli operator obtained through the double-partitioned scheme of Ref. [2]. There one has to define a core, given by the boundary $n_1$, which represents the last single-hole state. $n_2$ is the last single-particle state of the model space.

In the calculations of ZBJVM, the Pauli operator is defined as in (b) of Fig. 1. The model space is again limited by the boundary $n_2$, but we have no holes. This definition is the first step in the so-called “no-core” approach of Ref. [1]. In this work we use the Pauli operator in (b) of Fig. 1 and define the model space to consist of the 0s-, 0p-, 1s0d- and 1p0f-shells. We could then, in principle, use the corresponding $G$-matrix to obtain the eigenvalues within this model space. The authors of Ref. [1] are also interested in studying how important various model spaces are. They therefore calculate the eigenvalues with smaller spaces first (see Table I of Ref. [1]), say only the 0s-shell. However, they use the $G$-matrix defined with a model space which includes also the 0p-, the 1s0d- and the 1p0f-shells. In so doing, they have to include the ladder diagram of Fig. 2 and higher-order ladder diagrams as well, with intermediate states from the 0p-, 1s0d- and 1p0f-shells, since they use different model spaces in the calculations of spectra and the evaluation of the $G$-matrix, see e.g. the discussion in Ref. [2]. This is, to our knowledge, not done in Ref. [1]. Actually, we will demonstrate that the omission of these ladder diagrams explains to a large extent why ZBJVM obtain rather different results when they compare results from diagonalizations with one, two and three oscillator shells, respectively.

To demonstrate our point, we choose a fictitious system to consist of two particles only, and define various model spaces. The conclusions apply equally well to systems with more particles. Here we choose our hamiltonian $H$ to consist of

$$H = H_0 + G,$$

(2)

with the unperturbed single-particle energies which define $H_0$ given by the harmonic oscil-
lator

\[ \varepsilon_{nl} = \left(2n + l + \frac{3}{2}\right)\hbar\Omega + \Delta, \tag{3} \]

where \( \Omega \) is the oscillator energy. Here we set \( \hbar\Omega = 14 \) MeV. We add a negative shift \( \Delta = -71 \) MeV in order to obtain negative starting energies only (see the discussion in Section III) and use, as in Ref. [1], a fixed starting energy, chosen to be \(-100 \) MeV. This corresponds to twice the energy of a single particle state in the \( 0s \)-shell, a choice we made in order to avoid poles in the calculation of ladder diagrams. As will be discussed in the next section, the use of a fixed starting energy implies that we have a degenerate model space, which is rather questionable if the model space spans over several shells. The choice of a fixed starting energy is also done in order to avoid the problems with the non-hermiticity of the effective interaction discussed in Section IV. The parameters of the Bonn B potential in Table A.1 of Ref. [3] are used to define the nucleon-nucleon potential \( V \). The Pauli operator is defined as in (b) of Fig. [1], with \( n_2 \) given by the last single-particle state in the \( 1p0f \)-shell.

The resulting eigenvalues for the lowest lying \( JT = 10 \) state is shown in Table I. The most important components in the wave functions of this state arise from single-particle states in the \( 0s \)- and \( 0p \)-shells.

The results labelled \( G \), include only the \( G \)-matrix, as done in the work of ZBJVM. As can be seen from Table I, there is clearly a large difference (of the order of 50% or more) between results obtained with a model space defined by the \( 0s \)-shell only and a model space which includes all shells up to the \( 1p0f \)-shell. This qualitative pattern also agrees with Table I of ZBJVM. In their conclusions, Zheng et al. use this to infer that one needs to take into account large model spaces, since the binding energies do not stabilize as functions of the various model spaces\(^\text{[4]}\). We show in Table I that this conclusion is misleading. The results obtained with the \( G \)-matrix plus the two-particle ladder (2P) diagram up to third order in

\(^1\)Note that we omit any discussions on excited spectra, since these include in general more and more complicated configurations as one increases the model space.
$G$ (higher-order terms are negligible) for the 0s model space, show that these results are rather close to those obtained with $G$ for the model space which includes all four shells. This demonstrates clearly that the lack of stabilization in the calculation of the ground states in Ref. [1], is simply due to the omission of the particle-particle ladder diagrams.

Note that in our calculations with $G + 2P$ for more than one oscillator shell, we use a degenerate model space, as done by ZBJVM. This means that if define the model space to include the 0s-, 0p- and 1s0d-shells, all single-particle states have the same energy. This approximation explains also why the results of the $G + 2P$ calculations differ slightly from model space to model space. In this sense, the result obtained with the 0s-shell only, is the most rigorous one. This results shows also that low-order perturbation theory works well in reproducing the lowest $JT = 10$ state.

The results with $G$ should also have taken into account a non-degenerate model space, but here we have tried to follow ZBJVM as closely as possible. The problems with a non-degenerate model space are addressed in the next section.

**III. ROLE OF THE STARTING ENERGY**

In principle, the effective interaction should not depend on the choice of starting energy $\omega$, though, since an approximation to the perturbation expansion is made, the effective interaction may depend on $\omega$. In Table II of Ref. [1], it is shown that the excited spectra depend weakly on $\omega$, whereas the ground state of $^6\text{Li}$ depends strongly on $\omega$. This state varies from $-23.044$ MeV to $-29.366$ MeV with starting energies between $\omega = 20$ and $\omega = 38$, respectively. The authors of Ref. [1] give no physical arguments for why one should choose a given starting energy, except that certain starting energies give a better fit to the data.

The fact that they get more attraction with the largest starting energy is rather simple. With a positive $\omega$ we are closer to the poles in the energy denominator of $G$, i.e.

$$\frac{1}{\omega - H_0}.$$  (4)
However, the choice of a positive starting energy is not straightforward in the $G$-matrix calculation. With a negative starting energy (appropriate for the low-lying states of finite nuclei), there are no poles in the above energy denominator. Actually, a principle value integration should have been performed in the above calculation of $G$. This is however not our main objection against the use of the starting energy as a variable by ZBJVM. With a multi-shell model space, one can no longer use a fixed starting energy, rather, the starting energy should take into account the fact that the single-particle energies are no longer degenerate. As an example, consider the matrix element $\langle (0d_{5/2})^2 | G(\omega) | (0d_{5/2})^2 \rangle$ coupled to $JT = 10$. This matrix element would enter our multi-shell calculations in Table I. The correct starting energy should be the unperturbed energy of two particles in the $d_{5/2}$ orbit. This would correspond to $-44$ MeV in our example. This starting energy gives a matrix element of $0.20$ MeV. In the previous section we used a fixed starting energy of $-100$ MeV, which would give us a matrix element of $0.48$ MeV. Thus, if the other matrix elements behave in a similar way (and they do), the use of a degenerate model space as done by ZBJVM, becomes meaningless. A scheme which takes the starting energy dependence into account, was recently proposed by Suzuki et al. [4].

Thus, the starting energy is not a parameter which one can choose in order to obtain a good correspondence with the data. The dependence of $\omega$ must be taken into account in the calculations. However, this leads us to our last point, namely that of the non-hermiticity of the effective interaction. We have in our calculations used a fixed starting energy, in order to avoid this problem, which arises even at the level of the $G$-matrix.

**IV. NON-HERMITICITY OF THE EFFECTIVE INTERACTION**

In the first point we stressed the need of including the ladder diagram of Fig. 2. However, if one does this, a more serious problem arises, namely that of the non-hermiticity of the effective interaction. Assume now that the intermediate states in the two-particle ladder diagram are those of the 1s0d-shell only. Diagram (b) in Fig. 2 is then proportional to
\[-\frac{1}{4\hbar\Omega} \langle (0p)^2 \mid G \mid (1s0d) \rangle \langle (1s0d) \mid G \mid (0s)^2 \rangle, \quad (5)\]

where the intermediate states must be those of the 1s0d-shell if we use a model space for the effective interaction which consists of the 0s- and the 0p-shells. Ω is the oscillator frequency. The starting energy corresponds to the unperturbed energy of 0s-shell. If we now evaluate diagram (c), we get

\[-\frac{1}{2\hbar\Omega} \langle (0s)^2 \mid G \mid (1s0d) \rangle \langle (1s0d) \mid G \mid (0p)^2 \rangle, \quad (6)\]

which yields a strongly non-hermitian effective interaction. The starting energy corresponds here to the unperturbed energy of two particles in the 0p-shell. As done by ZBJVM, one could ignore ladder diagrams in the definition of the effective interaction, and thereby obtain a hermitian effective interaction in terms of \( G \) only\(^2\).

However, as discussed in Section II, if one truncates the model space, one has to include the ladder diagram, yielding a non-hermitian interaction. It is important to note that this non-hermiticity arises only if we approximate RS perturbation theory to a given order. If all terms are taken into account, this problem does not occur. Viable approaches to obtain an order-by-order effective interaction which is hermitian, have recently been proposed by Lindgren \[5\] and Kuo et al. \[6\].

This strong non-hermiticity is also present if one includes folded diagrams as well, as done in the recent work of Jaqua et al. \[7\]. The same critical remarks in the above Sections apply to that work as well.

\(^2\)In our \( G + 2P \) calculation in Section II we used a fixed starting energy, in order to avoid the non-hermiticity. Even with the \( G \)-matrix, the effective interaction will be non-hermitian if we do not use a fixed starting energy.
V. CONCLUSION

In summary, we have shown that the differences between results for various model spaces obtained by the authors of Ref. [1], is due to the omission of the particle-particle ladder diagrams in their calculations. Thus, the conclusion by ZBJVM, that the binding energies do not stabilize as functions of various model spaces, is not correct. Actually, we have demonstrated that low-order perturbation theory gives the same results within a small model space as the calculations in terms of the $G$-matrix in a large model space. Moreover, we argue that the use of a fixed starting energy by Zheng et al. may not be a viable approach, since the calculations involve several shells, and the starting energy should take this into account.

However, if one wishes to properly evaluate the starting energy dependence and include the ladder diagrams, one has to face the problem of the non-hermiticity of the effective interaction, since one is dealing with an interaction defined for several shells.

Finally, all such calculations, which involve many single-particle orbits from several shells, do become prohibitively time-consuming for all nuclei but the lightest ones. Thus, even with the present increased computing power, the perspectives for computing properties of more interesting systems like $^{18}$O, are rather meagre.
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FIGURES

FIG. 1. Two different choices for the Pauli operator $Q$ used in the calculation of the $G$-matrix. See text for further discussion.

FIG. 2. (a) is the two-particle ladder diagram to second order in the $G$-matrix (wavy line). (b) and (c) are examples of ladder diagram contributions with intermediate states from the $1s0d$-shell only.
TABLE I. Eigenvalues for a system with two particles for different model spaces. The second column lists the results for a model space consisting of the single-particle orbits of the 0s-shell only. The third column includes the 0p-shell while the fourth and fifth columns include the 1s0d- and 1p0f-shells, respectively. The row denoted by $G$ means that only the $G$-matrix defined in the text is used, while $G + 2P$ includes the two-particle ladder diagram to third order in $G$. The results are scaled so that $\varepsilon_{0s1/2} = 0$.

|       | 0s  | 0s − 0p | 0s − 1s0d | 0s − 1p0f |
|-------|-----|---------|-----------|-----------|
| $JT^\pi = 10^+$ |     |         |           |           |
| $G$   | -7.83 | -9.13   | -11.03    | -12.35    |
| $G + 2P$ | -12.37 | -12.33  | -12.30    | –         |
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