Effective interactions for dominant shell-model configurations: $ds$-shell example

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Starting from the $ds$-shell interaction of Kuo, orthogonal polynomial and Brillouin-Wigner expansions for effective interactions in the dominant configurations space for low-lying states of $^{90}$Zr, $^{92}$Zr, and $^{94}$Zr have been calculated. Although the states represented have no more than 2% of their strength in the model space, the orthogonal polynomial series converges in low order and good predictions can be obtained with only a third order theory, especially if self-consistency is required. For the Brillouin-Wigner expansions, however, we find that higher-order approximations ($\geq$ 5th order) are required to achieve reasonable accuracy for states lying below the lowest eigenvalue of the interaction in the excluded space. For higher-order states the Brillouin-Wigner self-consistent results diverge.

I. INTRODUCTION

Let $H = H_0 + V$ act in a full space with $H_0$ the unperturbed Hamiltonian and $V$ the residual interaction. An effective interaction satisfying the usual criteria and acting in a subspace $P$ of the full space can be written exactly as

$$V_{\text{eff}} = V - \frac{Q}{E - H_0} V,$$  \hspace{1cm} (1)

where $Q = 1 - P$ is a projection onto the excluded space and $H_0 = \text{GO}_Q$. The $P$ subspace is usually denoted the model space. It has been shown that a Rayleigh-Schrödinger (RS) perturbation expansion of (1) in powers of $V$ diverges whenever an "intrauder state" is present in the energy domain of the model space. \footnote{For a Brillouin-Wigner (BW) perturbation expansion it diverges whenever the energy $E$ lies above the lowest eigenvalue of $H_0$ or $\text{GO}_Q = H_0/H_0 - VQQ$.} But the divergence of these power series expansions does not necessarily imply the divergence of all polynomial series in the residual interaction. In spectral distribution studies this is well known for even though averages of powers of the Hamiltonian diverge with increasing order, shape parameters of a distribution, which are polynomial functions of these same moments, converge. \footnote{Therefore we suggested in Ref. 5 that Eq. (1) be expanded in terms of orthogonal polynomials (OP) associated with spectral configuration densities as} $V_{\text{eff}} = V = \sum \sum \sum \sum F_2^2(\mathbf{r})\mathbf{U}_{\mathbf{m},-\mathbf{m}}(\mathbf{r})\mathbf{U}_{\mathbf{m},-\mathbf{m}}(\mathbf{r})V$.  \hspace{1cm} (2)

In this "normal mode" expansion $W$ represents a configuration in the model space, $\mathbf{u}$ a configuration in the excluded space, $F_2^2(\mathbf{r})$ a 2nd order polynomial defined by the configuration density $\rho_2(\mathbf{r})$, and $F_2^2(\mathbf{E}) = \int \frac{\rho_2(\mathbf{r})}{E - E_{\text{cut}}} d\mathbf{r}$.  \hspace{1cm} (3)

In Ref. 6 we studied the convergence characteristics of this OP expansion using the modified Lippman model. We found that while for a strong perturbation the BW series diverges, the OP expansion converges. But because the dimensionality of the full space in that study was really much too small (5 and 7 for the two cases considered) to justify the assumed Gaussian form for configuration densities, inherent inaccuracies existed which weakened arguments regarding superiority of the OP leading approximation and the stability of its convergence. Here we report on results of a more realistic study, one selected because for it the Gaussian assumption is justified and exact results, which are necessary for an evaluation of the theory, can be generated with existing shell-model codes. Furthermore, it typifies a procedure that can be followed to both simplify and extend other shell-model investigations.

II. MODEL

In model studies one usually starts with $N$ nucleons distributed among a set of single-particle orbitals with the full space further defined by specifying the total angular momentum $J$ and isospin $T$. But for other than very light systems, such fixed-$J$ and $T$ spaces, even when the single-particle orbitals are restricted to one major oscillator shell, are often too large to be dealt with...
using existing shell-model codes and computational resources. Further truncation is not necessary and the model interaction, normally designed to be used in the full space, must be renormalized accordingly. Often this renormalization of the interactions is not done or only included phenomenologically by allowing, for example, single-particle energies to be adjusted. (Wong has suggested a procedure that scales classes of matrix elements so as to reproduce in the model space full space values for soft-core.) Partitioning the space by configurations leads to a natural and easy method for achieving both truncation and renormalization. For the $Q$ space one can pick one or several of the most important configurations and assign all others to the $Q$ space. The model-space effective interaction is then as given by (3). Partitioning according to irreducible representations of some special symmetry group, for example $SU_3$, may be preferred. However, the expansion for $V_{ef}$ is then more complex than that given in (2) for the $Q$ prediction only can be made effective via Racah reordering techniques. (See, for example, the discussion of blend of averages given in Ref. 4.)

With that as background we now turn to our six-shell example, $^{40}$Ca(1s-7s, 7p-0). The full space has dimensionality 307 and 32 configurations. For the unperturbed Hamiltonian, $H_0$, we have chosen $^{40}$Ca single-particle energies and for $F$ the 6-shell interaction of Rabi. For the $Q$ space we have chosen the single configuration $\sum_{\nu=1}^{3} a_{\nu} Y_{\nu}(\theta, \phi)$ which dominates the low-lying eigenstates. It has dimensionality 30 and includes 22 of the total 32 states below 54 MeV, the approximate energy of the 6th eigenstate as determined using Rabi's method. From the exact results, obtained by diagonalizing the interaction in the full space, we note that among the first five states only the 1st, 2nd, and 4th have strengths greater than 35% in the model space with actual values 31%, 23%, and 21%, respectively. The perturbation from the excluded space therefore is extremely strong. The third eigenstate is an intruder because for it the (41) configuration is not dominant with only a 9% strength.

II. RESULTS AND DISCUSSION

In Fig. 1(a) we have plotted the four lowest eigenenergies (solid horizontal lines) obtained when various OP approximations for $V_{ef}$ were renormalized in the model space. The index indicates the maximum order in $V$ included in the expansion of $V_{ef}$, 8th order theory. As in (2) we have $\nu_{max}=1$ with $\nu_{max}=1$ for $H_0$. Also plotted are the corresponding BW predictions (broken lines) as order-by-order contributions between the two can be easily made. On the far right the exact energies are given. In expanding $V_{ef}$, the value of $\nu$ was not exact to the first exact eigenenergy. Order-by-order approximations, indicated by the lines connecting levels, were determined from overlap $\langle \phi_{\nu} | \phi_{n} \rangle$ between eigenstates of neighboring approximations. Except for some low-order cases the overlap are usually greater than 90% in the approximated OP space. We also calculated normalized overlaps between the exact eigenstates $\langle \phi_{\nu} | \phi_{n} \rangle$ projected into the model space and the various approximations,

$$\langle \phi_{\nu} | \phi_{n} \rangle = \sum_{\nu=1}^{30} \langle \phi_{\nu} | \phi_{n} \rangle$$

(4)

Whenever this overlap exceeds 95%, the approximation has been labeled with the value (or 100% in parentheses) if it exceeds 90% the parentheses has been omitted. The results in Fig. 1(b) show that energies calculated with an OP theory of given order are better than the corresponding BW values. In particular, note that the OP leading approximation $\langle \phi_{\nu} | \phi_{n} \rangle > 0.9$ corrects the energies by more than twice the amount generated by the corresponding BW theory. This is as predicted in Ref. 5 but not observed in the Ligeti model study because the Gaussian assumption there was too severe. In fact, the OP leading approximations are better than the 4th order BW predictions and the 3rd order polynomial results with more than half the energy discrepancy between $H_0$ and $V_{ef}$ corrected are better than the all approximations $\langle \phi_{\nu} | \phi_{n} \rangle$ through the order shown in Fig. 1(a). Both leading approximations predict the lowest state correctly but the 2nd and 4th are inverted. Whereas the OP expansion corrects this in 3rd order, a 5th order BW theory is required. Wave functions of the OP series are also better representations of the true eigenstates than the corresponding BW results. A 3rd order OP theory produces overlaps with the 1st, 2nd, and 4th states exceeding 90% whereas that first occurs in 6th order for the BW expansion. The 4th model-space state has maximum overlap with the 12th exact eigenstate but not even in 7th order does this exceed 75%, though again the OP results are best.

All the results in Fig. 1(a) were obtained with $\nu_{max}=1$ equal to the first exact eigenenergy. This choice ensures convergence of the BW series because $K$ is below the lowest eigenvalues of $H_0$ and $V_{ef}$. The increasing inaccuracy of predictions for higher energy states that this choice produces (see the figure) gives an indication of the energy dependence of (1). We have also calculated the effective interaction for each state using the exact energy so disagreement, order by order, are due solely to the expansion technique. These
FIG. 1. (a) Plots of the lowest four eigenvalues of effective interactions in the dominant configuration $(\omega, I=1)$ for orthogonal polynomial (solid) and Brillouin-Wigner (dashed) expansions through order $Q=276$ in $\Omega$ which was taken to be the $\Delta$-shell interaction of Ref. 9. For $\langle \omega \rangle$, the unperturbed Hamiltonian, the single-particle eigenvalues of $Q_\Omega$ were used. For $\langle \omega \rangle$, the model-space eigenstates and so exact full-space eigenstate exceeds 99\%, the number of that exact eigenstate labels the level; if this is lower than 99\% but greater than 70\%, the number is enclosed in parentheses. On the far right the exact energies are indicated. (b) Plots of the lowest four eigenvalues of effective interactions for $\langle \omega \rangle$, the unperturbed Hamiltonian, with $\langle \omega \rangle$ of Eq. (2) set equal to the exact energy of the state represented. See (a) for details. (c) Plots of the lowest four eigenvalues of effective interactions for $\langle \omega \rangle$, the unperturbed Hamiltonian, with $\langle \omega \rangle$ of Eq. (2) set equal to the exact energy of the state represented. See (a) for details.

results are shown in Fig. 1(b). This choice for $\langle \omega \rangle$ improves the convergence of the excited state predictions, especially with low-order G0P results which now in 3rd order account for more than 60\% of the energy difference between $\langle \omega \rangle$ and $I_F$. Except for the 12th state, the changes in both predicted energies and overlaps are rather moderate, which is probably due to the fact that the exact energies are within 3 MeV of one another and are still below the lowest eigenvalue of $\langle \omega \rangle$ or $\bar{\Omega}_Q$. Note that for BW the 2nd–4th level inversion is not corrected until 7th order though the over-
large show slight improvement. For the 12th state the BW results do not show signs of convergence. Overlaps with the exact 12th state increase in low order but from 4th order to 7th order decrease from 70% to less than 50% while over the same range overlaps with the 3rd state increase from less than 40% to more than 70%. For this case the exact energy is above the lowest eigenvalue of $H_0$ and convergence is expected; the changing structure of the eigenstates signals this. However, just as in the lightest model study the OP results for the 12th state show convergence in low order and then hover about an average close to the exact value. Overlaps with the exact 12th state are persistently the largest, generally greater than 70% (65% in the 3rd and 4th order), in applications the exact energies are unknown and one must select a starting value; for example, a reasonable choice would be one determined using Batchel's prescription. One can certainly reduce the dependence on this choice by including more configurations in the model space. A better approach, but one that is more demanding to implement, is to require order-by-order self-consistency. In Fig. 3(b) we show the self-consistent solutions for the four lowest order consideration. The BW results improve a great deal, especially in higher orders where the energy correction is increased by as much as 50%. Overlaps now exceed 90% for the lowest three states in 7th order and the 2nd and 4th states are correctly ordered in 6th order. The OP results also improve with the most significant change in low orders. The 3rd order self-consistent OP expansion accounts for more than 70% of the energy difference between $H_0$ and $H$ and it is still better than the 7th order self-consistent BW theory. The OP overlaps remain high except the values for the 2nd state in 5th and 6th order decrease slightly to 60% BW are back up above 90% in 7th order. This is consistent with the slight oscillation one sees in the corresponding energy predictions. Results for the 4th state are much as in Fig. 3(b) with the OP results showing convergence and the BW results divergence.

IV. CONCLUSION

In summary, the results of this study demonstrate the superiority of an OP theory for generating model-space effective interactions in real nuclei. The energy dependence is not strong but can be used to advantage for requiring self-consistency leads to high accuracy in low order, even when the perturbation from the excluded space is strong. For the case studied a 2nd order self-consistent OP theory which includes only a configuration density weighting of quasibound terms in $V$ is almost equivalent to a 4th or 5th order self-consistent BW theory and a 3rd order OP theory, a realistic expectation for applications, yields results that are excellent, even better than 7th order BW predictions. In addition we have demonstrated that the OP series can converge in situations where the BW theory is known to diverge.

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