Perturbative Approach for the Ground-State Correlations of Vibrational Nuclei*

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An approximate procedure which makes use of the spherical Hartree-Fock method and the perturbation approximation is described for generating the correlated ground state. This procedure is compared with an exact shell-model method and with the projected Hartree-Fock (PHF) method, with or without time-reversal constraint, by studying the octupole correlations in O^{16}. It is shown that the results given by the present simple method are comparable with the more difficult PHF method with no time-reversal constraint.

I. INTRODUCTION

SEVERAL authors[1,2] have proposed renormalized random-phase-approximation (RPA) equations to calculate the excited states for vibrational nuclei. To apply these methods, a preliminary knowledge of the correlated ground state is needed. A number of methods have already been suggested by Rowe[3] to calculate the ground-state correlations. Recently, it has been shown[4–6] that one of the promising methods is the projected-Hartree-Fock (PHF) technique, in which one applies the variational principle after projecting out the ground state from an intrinsically deformed determinant. This method is interesting because it accounts for both vibrational and rotational correlations in a continuous manner, but it cannot include all types of correlations as long as one imposes symmetry constraints, e.g., the time-reversal constraint.[5,6] As shown in the present paper, much better results can be obtained when the time-reversal constraint is relaxed. Even though these PHF calculations can now be performed,[5,6] they are fairly difficult and use a large amount of computer time.[6] One therefore needs a much quicker and easier method to generate the approximate correlated ground state comparable with the one obtained by PHF. In this note, we would like to propose another approximate procedure which makes use of the spherical Hartree-Fock method and the perturbation approximation as described by Nesbet.[7] It was used earlier to calculate the correlation energy for the ground state of the O^{16} nucleus.[8] It will be shown that the correlated ground state generated by the present, much simpler, method, which unlike PHF takes into account all types of correlations, is as good as the one obtained by the more difficult PHF method even when the time-reversal constraint is relaxed.

In Sec. II, we describe the present method and show the results in Sec. III.

II. METHOD OF CALCULATION

Let Ψ be an exact wave function and Φ_0 its dominant component, then we can write

$$\Psi=\lambda[\Phi_0+\sum_{\mu\neq 0} a_\mu\Phi_\mu], \tag{1}$$

where λ is the normalization constant. The coefficients a_μ in the perturbation approximation[7] are given by

$$a_\mu=H_{\mu 0}/(H_{\mu\mu}-H_{00}), \tag{2}$$

where H is the Hamiltonian, and $H_{\mu\nu}=\langle\Phi_\mu \mid H \mid \Phi_\nu\rangle$. In practical applications,[8] Φ_0 is first taken to be the dominant shell-model wave function and the coefficients a_μ are calculated using expression (2). If some of the coefficients a_μ turn out to be large, then the Hamiltonian is exactly diagonalized in the basis set consisting of Φ_0 and those Φ_μ for which the coefficients a_μ were large. This then defines a new Φ_0, and the coefficients are recalculated using expression (2). In the closed-shell nuclei like O^{16}, there is a big gap between the occupied and the unoccupied spherical Hartree-Fock orbitals,[8,9] and therefore the size of the Hamiltonian matrix which has to be diagonalized exactly is quite small.

Let us now apply this method to calculate the correlated ground state of O^{16}. Since our aim here is to compare the results of the present method with the PHF and the exact shell-model results, we shall use the same interaction and configuration space which we had used earlier.[5] The configuration space is limited to four nucleons in the $1p_{1/2}$ and $1d_{5/2}$ subshell outside of a $(1s_{1/2})^4(1p_{3/2})^8$ closed-shell core. The two-body

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interaction is taken to be the Rosenfeld interaction

$$V(r)=\tfrac{1}{3}V_0\tau_1\cdot\tau_2(0.3+0.7\sigma_1\cdot\sigma_2)e^{-\mu r}/\mu r, \quad (3)$$

with $V_0=50$ MeV, $\mu^{-1}=1.37$ fm. The single-particle energies $\epsilon_{p1/2}$ and $\epsilon_{d5/2}$ are -4.95 and -1.10 MeV, respectively. To see the effects of the octupole correlations, an octupole-octupole interaction

$$v=-\chi r_1^2 r_2^2 \sum_q Y_{3q}(\theta_1)\,Y_{3q}^*(\theta_2) \quad (4)$$

is artifically added to the Hamiltonian.[5]

The quantities of interest are the correlation energies ΔE,

$$\Delta E=\langle\Psi_{0^+}\mid H\mid\Psi_{0^+}\rangle-\langle(p_{1/2})^4\mid H\mid(p_{1/2})^4\rangle, \quad (5)$$

and the single-particle densities for the ground state of O^{16}. These quantities were calculated[5] using the PHF technique with the time-reversal constraint as a function of the strength of the octupole-octupole interaction, and then compared with the corresponding exact shell-model results. By choosing χ to be both positive and negative, the effects of suppression and enhancement of the octupole correlations on the correlation energy and single-particle densities were studied.[5] We show in Sec. III how these quantities change when the time-reversal constraint is relaxed and how they compare with the ones given by the approximate perturbation procedure.

III. RESULTS AND DISCUSSIONS

The approximate perturbation procedure is applied both to the ground state $J^\pi=0^+$, $T=0$ and the low-lying excited state $J^\pi=3^-$, $T=0$ of the O^{16} nucleus. For both these states we had to diagonalize exactly a 2×2 matrix and all the remaining a_μ coefficients were calculated using expression (2). Instead of calculating the single-particle densities in the ground state and the octupole transition matrix, we have calculated the overlaps of our approximate $J^\pi=0^+$, $T=0$ and $J^\pi=3^-$, $T=0$ wave functions with the corresponding exact shell-model wave functions and have tabulated them in Table I. The values of the correlation energy ΔE for the ground state and the energy of the low-lying 3^- state calculated using the present method are also shown in Table I. For comparison the exact shell-model results and the PHF results obtained with the time-reversal constraint are also given in the same Table.

Before we compare the results given in Table I, we remark that the ground state of O^{16} has been calculated by a number of authors using various approximation procedures. One such study has been carried out recently by Ellis and Zamick.[10] They have

[10] P. J. Ellis and L. Zamick, in *International Conference on Properties of Nuclear States, Montreal, 1969* (University of Montreal Press, Montreal, 1969), Contribution No. 7.22.

TABLE I. Correlation energy ΔE, energy of the $J^\pi=3^-$, $T=0$ state relative to the ground state, and the overlaps with the shell-model (s.m.) wave functions. For convenience χ is expressed in the units of 0.0364 fm^{-4}.

	Shell model		PHF (with time-reversal constraint)				Present method			
χ	$-\Delta E$ (MeV)	E_{3^-}, $T=0$ (MeV)	$-\Delta E$ (MeV)	E_{3^-}, $T=0$	$\langle\Psi_{0^+}^{\rm PHF}\mid\Psi_{0^+}^{\rm s.m.}\rangle$	$\langle\Psi_{3^-}^{\rm PHF}\mid\Psi_{3^-}^{\rm s.m.}\rangle$	$-\Delta E$ (MeV)	E_{3^-}, $T=0$	$\langle\Psi_{0^+}^{\rm P}\mid\Psi_{0^+}^{\rm s.m.}\rangle$	$\langle\Psi_{3^-}^{\rm P}\mid\Psi_{3^-}^{\rm s.m.}\rangle$
−6	0.6555	5.6887	0.2548	5.4213	0.9858	0.9957	0.6527	5.6877	0.9999	0.9999
−5	0.8566	5.4475	0.4928	5.2090	0.9868	0.9959	0.8561	5.4489	1.0000	0.9999
−4	1.1449	5.2440	0.8246	5.0403	0.9901	0.9962	1.1440	5.2451	1.0000	0.9999
−3	1.5266	5.0842	1.2539	4.9185	0.9916	0.9966	1.5201	5.0801	0.9997	0.9999
−2	2.0040	4.9724	1.7786	4.8441	0.9931	0.9969	1.9850	4.9563	0.9992	0.9999
−1	2.5756	4.9097	2.3928	4.8165	0.9943	0.9970	2.5363	4.8740	0.9984	0.9999
0	3.2359	4.8946	3.0843	4.8322	0.9950	0.9968	3.1688	4.8317	0.9974	0.9999
1	3.9771	4.9229	3.8426	4.8704	0.9965	0.9975	3.8759	4.8270	0.9962	0.9998
2	4.7900	4.9898	4.6958	4.9728	0.9974	0.9975	4.6500	4.8563	0.9950	0.9998
3	5.6643	5.0896	5.5778	5.0814	0.9972	0.9977	5.4833	4.9161	0.9939	0.9998
4	6.5917	5.2171	6.5327	5.2319	0.9986	0.9976	6.3684	5.0026	0.9928	0.9997
5	7.5640	5.3677	7.4995	5.3752	0.9980	0.9979	7.2984	5.1126	0.9920	0.9997
6	8.5743	5.5374	8.5380	5.5844	0.9992	0.9972	8.2673	5.2428	0.9912	0.9996

TABLE II. Correlation energy ΔE and the overlap of the improved PHF ground-state wave function Ψ_0^+ of O^{16}, obtained without any time-reversal constraint, with the corresponding shell-model wave function.

χ	$-\Delta E$ (MeV)	$\langle \Psi_0^{+\mathrm{PHF}} \mid \Psi_0^{+\mathrm{s.m.}} \rangle$	χ	$-\Delta E$ (MeV)	$\langle \Psi_0^{+} \mid \Psi_0^{+\mathrm{s.m.}}$
−6	0.6467	0.9998	1	3.8974	0.9978
−5	0.8462	0.9997	2	4.7752	0.9996
−4	1.1337	0.9997	3	5.6504	0.9997
−3	1.5134	0.9997	4	6.5784	0.9997
−2	1.9898	0.9996	5	7.5514	0.9997
−1	2.5603	0.9996	6	8.5619	0.9997
0	3.2204	0.9996			

also made use of the perturbation theory, but with the difference that their Φ_0 is restricted to a 0-particle–0-hole state and all the other Φ_μ are then necessarily restricted to 2-particle–2-hole states because of the two-body nature of the interaction. This straightforward use of the perturbation theory has been used in the past by a number of other authors, whereas in the present general approach, Φ_0 is not restricted to the single shell-model component, and thus, Φ_μ have the possibility of including, for example, 4-particle–4-hole components also. Since the objective of Ellis and Zamick is to calculate the 2-particle–2-hole admixtures in the ground state, they have used a much larger configuration space than the one used here.

The aim of the present calculation, as mentioned in the Introduction, is to generate a perturbative correlated ground state to use in the equations-of-motion calculations.[5,6] It has been shown[4–6] that the PHF method, even though difficult in practice, gives a fairly satisfactory correlated ground state for this purpose. This state not only contains 2-particle–2-hole components, but also all the other $2n$-particle–$2n$-hole components. It is easy to see that the perturbative procedure described in Sec. II can produce such a state and, as shall be shown shortly, this correlated state is better than the one obtained by the PHF method with the time-reversal constraint. Even when the time-reversal constraint is relaxed in the PHF method to obtain a better wave function, the perturbative wave function still compares nicely with it.

The other advantage of the present method is that if there are several Φ_μ with amplitudes comparable with the single shell-model wave function Φ_0, then they can be easily taken care of by the exact diagonalization in this small set to define a new Φ_0.[8] For example, in the present calculation Φ_0 is obtained by diagonalizing a 2×2 matrix.

The present procedure is applied to O^{16} as an example, since the PHF results with the time-reversal constraint are already known for this case.[5] Not only the 0^+, but also the 3^- state is calculated by the present method and compared with the exact shell model and the PHF results, both with and without the time-reversal constraint. By studying the problem as a function of the octupole deformation parameter χ, the validity of the present perturbative approach is checked for a wide range of octupole correlations.

We now go back to Table I and compare the results of the present calculation with those of the shell model and the PHF with the time-reversal constraint. We find that, except in the large octupole correlation region, the approximate correlated ground-state wave function calculated by the much simpler present method is better than the one given by PHF using time-reversal constraint.

As mentioned earlier, the perturbation method includes all correlations, whereas the constrained PHF does not. This is demonstrated by relaxing the time-reversal constraint and observing the improved PHF results, which are shown in Table II.

On comparing the results of the present method, given in Table I, with the results obtained by the PHF method relaxing the time-reversal constraint given in Table II, we find that the present method gives as good results as the PHF method without the time-reversal constraint, and can therefore be used as a quicker and easier method to generate the approximate correlated ground state.

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