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Quasi-Spin Projection in an Exactly Soluble Model*

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An exactly soluble model for the study of projection techniques within the framework of the Hartree-Fock theory is presented. Properties of the exact solutions are analyzed and projections, both before and after variation, are discussed.

1. Introduction

One often utilizes in nuclear physics ground state wave functions which are not eigenstates of a given operator $\hat{O}$, even if that contradicts physical requirements involving the conservation of the observable represented by $\hat{O}$. It is well known [1] that Hartree-Fock (HF) selfconsistent solutions generally correspond to situations in which either the center-of-mass linear momentum or the total angular momentum (or both) is not a well-defined observable. Literature on the subject has been growing during the last years (see for example Refs. 2), and, in particular, angular momentum projection has received a great deal of attention (see for instance Ref. 3 and works cited therein).

When projection techniques are employed in a given calculation, approximations at different levels, are usually made, specially if projection-before-variation is intended [4–6]. It is not always an easy task to ascertain to what an extent these approximations are valid ones, since no exact wave functions are in most cases available. For this reason, exactly soluble models are of special usefulness. In this respect, the most widely used model of this type is perhaps Lipkin's one [7, 8]. Although extremely useful in many situations, this model is not particularly helpful in dealing with projection techniques, as only parity can be projected out [8, 9].

The purpose of the present work is to present an exactly soluble model which, although only slightly more involved than Lipkin's, is specially suited to study projection techniques. Moreover, a richer structure is found, in the sense that several "phase transitions" are encountered.

The model is introduced in Sect. 2, while the corresponding HF solutions are dealt with in Sect. 3. Projection theory, both before and after variation, illustrated with numerical results, is discussed in Sects. 4 and 5.

2. The Model

The model deals with N particles distributed in two single-particle levels, each N-fold degenerate, which are separated by the single particle energy ε. We characterize the N lower states by $|p, \sigma = -1\rangle$ (for $p = -\frac{N}{2}, \ldots, N/2$) as Lipkin et al. [7, 8]. The particles interact via a two-body force of strength V_s, whose structure is a bit more complicated than that of Lipkin's monopole force. The Hamiltonian reads

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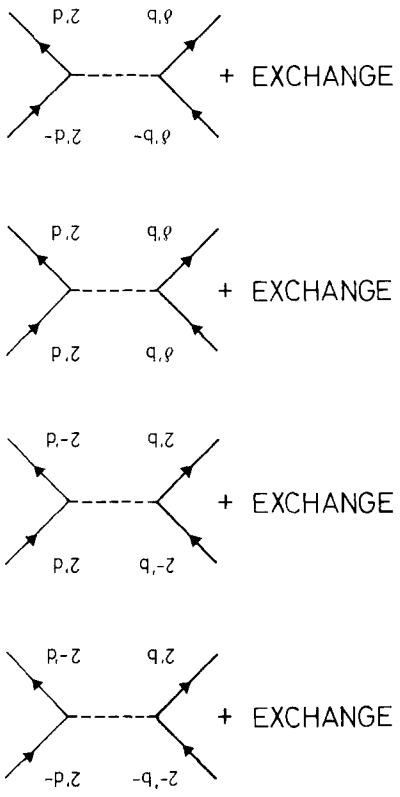

Fig. 1. Interaction diagrams entering the model's Hamiltonian

$$\hat{H}=\tfrac{1}{2}\varepsilon\sum_{p\mu}\mu c^{\dagger}_{p,\mu}c_{p,\mu}$$
$$+\tfrac{1}{2}V_s[\tfrac{1}{8}\sum_{pq\sigma\tau}\sigma\tau c^{\dagger}_{p,\sigma}c^{\dagger}_{q,\tau}(c_{q,\tau}c_{p,\sigma}-c_{-q,\tau}c_{-p,\sigma})$$
$$+\tfrac{1}{4}\sum_{pq\mu}c^{\dagger}_{p,\mu}c^{\dagger}_{q,-\mu}(c_{q,\mu}c_{p,-\mu}-c_{-q,\mu}c_{-p,-\mu})]. \tag{1}$$

As depicted in Fig. 1, four different interaction terms are included in the Hamiltonian (1), both repulsive and attractive. In order to study its properties it is convenient to introduce, in addition to the usual [7, 8] quasi-spin operators

$$\hat{J}_z=\tfrac{1}{2}\sum_{p\mu}\mu c^{\dagger}_{p,\mu}c_{p,\mu},$$
$$\hat{J}_+=\hat{J}^{\dagger}_-=\sum_p c^{\dagger}_{p,+}c_{p,-}, \tag{2}$$

the following ones

$$\hat{S}_+=\hat{S}^{\dagger}_-=\sum_p c^{\dagger}_{p,+}c_{-p,-},$$
$$\hat{S}_z=\hat{J}_z. \tag{3}$$

The operators $\hat{S}_+$, $\hat{S}_-$, $\hat{S}_z$ commute among themselves like angular momentum ones, i.e., they are quasi-spin operators.

If we define further

$$\hat{U}=\tfrac{1}{2}\sum_{p,\mu}\mu c^{\dagger}_{p,\mu}c_{-p,\mu}, \tag{4}$$

and

$$\hat{V}_+=\hat{V}^{\dagger}_-=\tfrac{1}{2}(\hat{J}_+ +\hat{S}_+),$$
$$\hat{W}_+=\hat{W}^{\dagger}_-=\tfrac{1}{2}(\hat{J}_+ -\hat{S}_+),$$
$$\hat{V}_z=\tfrac{1}{2}(\hat{J}_z+\hat{U}),$$
$$\hat{W}_z=\tfrac{1}{2}(\hat{J}_z-\hat{U}), \tag{5}$$

we obtain two additional quasi-spin sets: $\hat{V}_+$, $\hat{V}_-$, $\hat{V}_z$ and $\hat{W}_+$, $\hat{W}_-$, $\hat{W}_z$. Moreover, any given $\hat{V}$ operator commutes with all $\hat{W}$ ones and viceversa ($SU_2\times SU_2$).

In terms of these new operators, we can write the Hamiltonian (1) as

$$\hat{H}=\hat{J}_z+\tfrac{1}{2}v(\hat{T}_1+\hat{T}_2), \tag{6}$$

with

$$\hat{T}_1=2\hat{V}_z\hat{W}_z,$$
$$\hat{T}_2=\hat{W}_+\hat{V}_-+\hat{W}_-\hat{V}_+. \tag{7}$$

In (6) we have defined $v=V_s/\varepsilon$. Obviously, we can diagonalize $\hat{H}$ in an $SU_2\times SU_2$ basis. Since $\hat{H}$ commutes both with $\hat{V}^2$ and $\hat{W}^2$, exact solutions are obtained by diagonalization within a given multiplet $|V,W,V_z,W_z\rangle$. It is easy to show that the following relationships hold.

$$\hat{J}^2=\hat{V}^2+\hat{W}^2+\hat{T}_1+\hat{T}_2, \tag{9}$$
$$\hat{S}^2=\hat{V}^2+\hat{W}^2+\hat{T}_1-\hat{T}_2. \tag{10}$$

As a consequence of (6) and (9), our Hamiltonian commutes with $\hat{J}^2$ but not with $\hat{S}^2$.

Let us discuss now the unperturbed ground state and denote it as $|\text{ugs}\rangle$. Obviously

$$\hat{J}_z|\text{ugs}\rangle=-\tfrac{1}{2}N|\text{ugs}\rangle,$$
$$\hat{U}|\text{ugs}\rangle=0. \tag{11}$$

Consequently, $|\text{ugs}\rangle$ is an eigenstate of both $\hat{V}_z$ and $\hat{W}_z$ with eigenvalues $V_z=W_z=-N/4$. Moreover,

$$\hat{V}^2|\text{ugs}\rangle=\hat{W}^2|\text{ugs}\rangle=\frac{N}{4}\left(\frac{N}{4}+1\right)|\text{ugs}\rangle, \tag{12}$$

i.e., the unperturbed ground state belongs to the multiplet $V=W=N/4$ and can be written as

$$|\text{ugs}\rangle=|V=W=N/4,V_z=W_z=-N/4\rangle. \tag{13}$$

Since $\hat{H}$ commutes both with $\hat{V}^2$ and with $\hat{W}^2$, the exact wave function must be a linear combination of

states pertaining to this multiplet. Moreover, in view of (9), we can label the exact solutions with the quasi-spin J and write down the energy explicitly as

$$E_{J,N}(V=W=N/4) = -J+\tfrac{1}{2}v[J(J+1)-2W(W+1)], \quad (14)$$

with $J \leqq N/2$.

If we focus now our attention upon the energy difference between two states of given N, and such that the corresponding quasi-spins J differ by one (i.e., they are, respectively, $J-1$ and J), we find

$$E_{J-1,N}-E_{J,N}=1-Jv \quad (15)$$

independent of N. One thus gets a set of "critical" coupling constants

$$v_J=1/J. \quad (16)$$

At $v=v_J$, the Lipkin quasi-spin of the ground state changes. In particular, for $v>1$, the ground state of the interacting system is characterized by $J=0$, independent of N. We see then that, as we turn the interaction on, the ground state of the system (which for $v=0$ possesses the maximum possible quasi-spin J compatible with N) will run downward in J as v grows, passing through all possible values until it reaches $J=0$ at $v=1$.

3. The Hartree-Fock Solution

The Hartree-Fock approach looks for the zero particle-zero hole ($0p-0h$) wave function in the selfconsistent or "b" representation, which is a suitable linear combination of the original, or "c", one. The corresponding coefficients are so chosen as to minimize the expectation value of the Hamiltonian in the new $0p-0h$ state. A glance at Fig. 1 should convince the reader that, in order to obtain the HF transformation one must mix the single-particle orbital $|p,\mu\rangle$ both with $|p,-\mu\rangle$ and $|-p,\mu\rangle$. This is conveniently done in two steps, i.e., one performs the two successive rotations [10, 11].

$$\begin{pmatrix} c_{-p,-} \\ c_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\beta/2 & -i\sin\beta/2 \\ -i\sin\beta/2 & \cos\beta/2 \end{pmatrix} \begin{pmatrix} a_{-p,-} \\ a_{p,+} \end{pmatrix}, \quad (17)$$

and

$$\begin{pmatrix} a_{p,-} \\ a_{p,+} \end{pmatrix} = \begin{pmatrix} \cos\alpha/2 & -i\sin\alpha/2 \\ -i\sin\alpha/2 & \cos\alpha/2 \end{pmatrix} \begin{pmatrix} b_{p,-} \\ b_{p,+} \end{pmatrix}. \quad (18)$$

The former is a rotation in quasi-spin S-space which commutes with $\hat{S}^2$ but not with $\hat{J}^2$, while the latter is a rotation in quasi-spin J-space, with the opposite behaviour. As a result of (17) and (18) both the V-quasi-spin and the W-one rotate around the x-axis, the former in an angle $(\alpha+\beta)$, the latter according to $(\alpha-\beta)$. The eigenvalues of both $\hat{V}^2$ and $\hat{W}^2$ are preserved in these rotations.

It is worthwhile to mention the following point. If we look at Fig. 1 we notice that, as we switch the interaction on, starting from the unperturbed ground state, only the forward (plus exchange) scattering term becomes effective, since there are no particles in the levels characterized by $\mu=+1$. Consequently, for small enough values of the interaction strength, the HF solution should match the exact one. In the Lipkin model, instead, things are quite different, since the HF solution deviates from the exact one as soon as the interaction is switched on [8]. Moreover, the Lipkin HF energy is independent of the coupling constant, as long as this is small enough. In our case, the HF energy depends *always* upon the interaction strength.

In order to determine α and β, and thus the $0p-0h$ state in the b-representation, we must solve the equations

$$\frac{\partial}{\partial\alpha}\langle \mathrm{HF}(b)|\hat{H}|\mathrm{HF}(b)\rangle=0,$$

$$\frac{\partial}{\partial\beta}\langle \mathrm{HF}(b)|\hat{H}|\mathrm{HF}(b)\rangle=0. \quad (19)$$

Table 1 lists the corresponding solutions. Notice that for the unperturbed ground state the exact energy is

$$E(|\mathrm{ugs}\rangle)=-\frac{N}{2}\left(1-\frac{vN}{8}\right), \quad (20)$$

which is also the HF energy for the trivial solution $\alpha=0$, $\beta=0$.

By inspection of Table 1 one concludes that the solution with $\alpha=\beta=0$ is the lowest one for $v<1/(2W)$, while for larger values of the coupling constant the unperturbed ground state becomes unstable and the solution $\alpha=0$, $\beta=\arccos\left(\frac{1}{2vW}\right)$ is the one to be selected. At this point, it is appropiate to refer again

Table 1. Values of the rotation angles α and β which extremalize the Hartree-Fock energy

α	β	HF energy
$\pi/2$	$\pi/2$	$-vW^2$
0	0	$-2W+vW^2$
0	π	$2W+vW^2$
π	0	$2W+vW^2$
0	$\arccos(1/2vW)$ (for $v>1/2W$)	$-(1/2v)-vW^2$

to the Lipkin model. There, a similar behaviour obtains, and an abrupt transition is exhibited by the HF energy at the critical coupling constant [8]. However, this is not the consequence of any physical effect, since the exact solution displays everywhere a smooth behaviour as a function of the interaction strength: In our case things are different. For our critical coupling constant there is a real phase transition, which is seen in the exact solution. Moreover, this phase transition is connected with the fact that, at that critical value, the attractive terms of the interaction overcome the effect of the repulsive ones.

As in Refs. 8, 10, 11, which deal with the Lipkin model, one can easily obtain an explicit expression for the HF wave function, in terms of the states of our relevant multiplet.

$$|\mathrm{HF}\rangle = \sum_{V_z W_z} D(V_z, W_z)\,|V, W, V_z, W_z\rangle, \tag{21}$$

with

$$D(V_z, W_z) = d^{V}_{-V, V_z}(\beta)\, d^{W}_{-W, W_z}(-\beta), \tag{22}$$

where the d functions are defined by Edmonds [12].

4. Exact Projection Theory

The HF wave-function (21) does not possess good quasi-spin J, although $|\hat{H}, \hat{J}^2| = 0$. In order to project out this quantum number it is convenient to diagonalize $\hat{J}^2$ within our relevant multiplet, this procedure yielding the set of wave functions.

$$|V, W, J, n\rangle = \sum_{V_z W_z} \mathscr{C}_{J,n}(V_z, W_z)\,|V, W, V_z, W_z\rangle. \tag{23}$$

Here n distinguishes among states of the same J. The set (23) allow us to give the projection operator $\hat{P}_J$ an explicit expression

$$\hat{P}_J = \sum_n |V, W, J, n\rangle\langle n, J, W, V|. \tag{24}$$

We see now that Eqs. (21–24) allow us to obtain an *exact* expression for the projected energy $E_J(\mathrm{PHF})$

$$E_J(\mathrm{PHF}) = \frac{\langle \mathrm{HF}|\,\hat{H}\hat{P}_J\,|\mathrm{HF}\rangle}{\langle \mathrm{HF}|\,\hat{P}_J\,|\mathrm{HF}\rangle}, \tag{25}$$

in terms of the wave functions of the multiplet $|V, W, V_z, W_z\rangle$, i.e., in terms of the matrix elements $\langle V, W, V_z', W_z'|\,H\,|V, W, V_z, W_z\rangle$, which have a very simple form.

Projection *after* variation is performed by using in (22), for β, the corresponding HF value of Table 1.

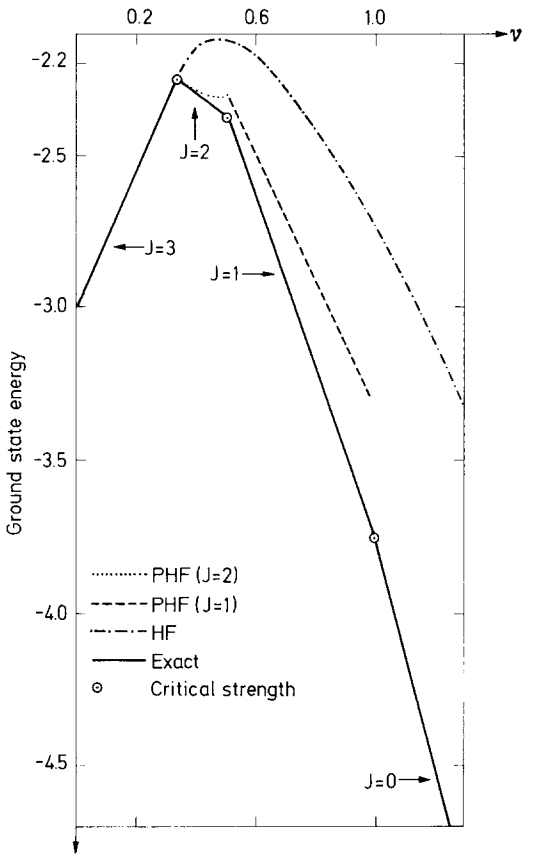

Fig. 2. Exact, J-projected and HF-energies for $N=6$. For $J=3$ the exact and HF energies coincide. For $J=0$ the exact and the PHF energies are equal. For $J=1,2$ projection before variation yields the same results as the exact treatment

Projection *before* variation is achieved selecting β in (22) so as to minimize (25).

Notice that for $v < 1/2W$ the HF solution has good J, since it coincides with the exact one. In projecting $J=0$, the following considerations should be made. There are $N/2+1$ states with $V_z = -W_z$ ($J_z = 0$) in the $|\mathrm{ugs}\rangle$-multiplet. Accordingly, $\hat{P}_0$ in (24) has only one term, and the projected energy coincides with the exact one, irrespective of wether one projects either before or after variation (the result does not depend upon β).

Figure 2 illustrates these considerations for the case $N=6$. As the strength v grows, the ground state of the system runs through several "phase transitions", where its Lipkin quasi-spin J changes abruptly at specific v_J values. For $J=3$ the exact solution is matched by the HF one. When $J=0$, the PHF solution coincides with the exact one, while the HF energy lies considerably higher. For $J=1,2$ one can appreciate the fact that projecting out J considerably improves the HF solution. Projection *before* variation yields the same results as the exact treatment,

Table 2. Overlaps between either the exact or the projected HF wave function and $|np-nh\rangle$, for $N=4$, $J=1$

v	$\lvert\langle \mathrm{HF}\rvert\mathrm{Exact}\rangle\rvert^2$	$\lvert\langle 1p\,1h\rvert\mathrm{Exact}\rangle\rvert^2$	$\lvert\langle 2p\,2h\rvert\mathrm{Exact}\rangle\rvert^2$	$\lvert\langle 3p\,3h\rvert\mathrm{Exact}\rangle\rvert^2$	$\lvert\langle 4p\,4h\rvert\mathrm{Exact}\rangle\rvert^2$
0.55	0.158	0.609	0.215	0.017	0.000
0.60	0.257	0.373	0.318	0.049	0.002
0.65	0.319	0.227	0.363	0.086	0.005
0.70	0.360	0.135	0.375	0.120	0.010
0.75	0.386	0.077	0.370	0.151	0.016
0.80	0.402	0.041	0.358	0.178	0.021
0.85	0.412	0.020	0.340	0.201	0.028
0.90	0.419	0.007	0.320	0.220	0.034
0.95	0.421	0.002	0.301	0.237	0.040
1.00	0.422	0.000	0.282	0.250	0.047
v	$\lvert\langle \mathrm{HF}\rvert\mathrm{PHF}\rangle\rvert^2$	$\lvert\langle 1p\,1h\rvert\mathrm{PHF}\rangle\rvert^2$	$\lvert\langle 2p\,2h\rvert\mathrm{PHF}\rangle\rvert^2$	$\lvert\langle 3p\,3h\rvert\mathrm{PHF}\rangle\rvert^2$	$\lvert\langle 4p\,4h\rvert\mathrm{PHF}\rangle\rvert^2$
0.55	0.158	0.618	0.194	0.027	0.001
0.60	0.259	0.396	0.261	0.077	0.008
0.65	0.325	0.261	0.270	0.124	0.021
0.70	0.370	0.176	0.253	0.162	0.039
0.75	0.401	0.122	0.228	0.190	0.059
0.80	0.424	0.086	0.201	0.209	0.081
0.85	0.440	0.062	0.175	0.220	0.104
0.90	0.453	0.045	0.151	0.226	0.126
0.95	0.461	0.033	0.130	0.227	0.148
1.00	0.469	0.025	0.113	0.224	0.169

and is thus seen to be a much more powerful method than projection *after* variation.

A numerical estimation of the correlations introduced by the projection procedure, which allows one to appreciate in greater detail the difference between these two methods, is obtained by evaluation of the overlap between either the exact, or the projected HF, wave function, and the state built upon the HF one by creating n particles and n holes $(np-nh)$, with $n=0,1,2,\ldots,N$. This can be accomplished by expansion of all relevant wave functions in terms of our basic set $|V,W,V_z,W_z\rangle$, as, for example, in Eq. (21) for the $0p-0h$ state. The procedure is straightforward, although the algebra involved may become cumbersome. In order to save space, we present in Table 2 just a representative example, for the case $N=4$, $J=1$.

An important conclusion that can be drawn from this study is that, qualitatively, projecting either before or after variation introduces the same kind of correlations. Only the relative weights of the different $np-nh$ corrections are different (remember that in this model projection before variation is equivalent to an exact solution).

There is also a strong correlation, as expected, between the goodness of the HF wave function and the importance of the $1p-1h$ admixtures in the exact wave functions. The best HF wave functions obtain when this admixture is zero. Curiously enough, this happens just at the critical strength that indicates the appearance of a phase transition.

5. Approximate Projection Theory

The most widely employed approximation is the so-called Gaussian overlap one (GOA) [3, 4]. In our context, application of the GOA is not straightforward, due to the fact that our HF states do not have good J_z. This difficulty can be surmounted by recourse to the expansions referred to in the last paragraph, i.e.

$$|np-nh\rangle=\sum_{V_z,W_z}\mathscr{C}_{np-nh}(V_z,W_z)\,|V,W,V_z,W_z\rangle. \tag{26}$$

For $n=0$ we have $\mathscr{C}_{np-nh}(V_z,W_z)=D(V_z,W_z)$ (see Eq. 21) and we have to consider up to $n=2$.

One must evaluate, then, the matrix elements (see Ref. 3 for notational conventions)

$$\begin{aligned}&\langle V,W,V_z,W_z|\,\hat{P}^{J}_{K}\,|V,W,V'_z,W'_z\rangle\\&=\langle V,W,V_z,W_z|\,\hat{p}_K\hat{Q}_{JKK}\hat{p}_K\,|V,W,V'_z,W'_z\rangle\\&=\delta_{K,V_z+W_z}\delta_{K,V'_z+W'_z}\langle V,W,V_z,W_z|\,\hat{Q}_{JKK}\,|V,W,V'_z,W'_z\rangle\end{aligned} \tag{27}$$

where

$$\hat{Q}_{JKK}=\tfrac{1}{2}(2J+1)\int_{-1}^{1}d(\cos\theta)\,d^{J}_{KK}(\theta)\,e^{-i\hat{J}_y\theta}. \tag{28}$$

For the sake of simplicity, let us choose $K=-J$. Then we have $d^J_{-J,-J}(\theta)=\left(\cos\frac{\theta}{2}\right)^{2J}$ and write

$$\langle V,W,V_z,W_z|\hat{Q}_{J,-J,-J}|V,W,V_z',W_z'\rangle$$
$$=\tfrac{1}{2}(2J+1)\int_{-1}^{1}d(\cos\theta)\left(\cos\frac{\theta}{2}\right)^{2J}$$
$$\cdot\langle V,W,V_z,W_z|e^{-i\hat{J}_y\theta}|V,W,V_z',W_z'\rangle. \quad (29)$$

The GOA is used in order to evaluate the matrix element in the r.h.s. of Eq. (29). One can use to that effect the expression (15) of Ref. 4 with the additional difficulty, in our case, that the index denoted there by s can here adopt values larger than 2.

The projected energy that is obtained in this way (see Ref. 4)

$$E_J=\langle \mathrm{HF}|\hat{H}|\mathrm{HF}\rangle+(2\langle \mathrm{HF}|\hat{P}_J|\mathrm{HF}\rangle)^{-1}$$
$$\cdot\sum_{L=|np-nh\rangle}\langle \mathrm{HF}|\hat{P}_J|L\rangle\langle L|\hat{H}|\mathrm{HF}\rangle$$
$$+\langle \mathrm{HF}|\hat{H}|L\rangle\langle L|\hat{P}_J|\mathrm{HF}\rangle \quad (30)$$

must now be minimized with respect to the angle β of Eq. (17). Numerical computations yield the result that, within numerical accuracy, GOA results coincide with those obtained by employing Eq. (30) without recourse to this approximation (which in turn, as previously discussed, are just the exact ones). We remark that, obviously, the GOA is an approximate projection before variation method. The conclusion to be drawn from our results is that an approximate projection before variation method is better than an exact projection after variation.

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