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Dynamical Basis Generation and Structure of the Hartree-Fock Approximation

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A variational method is developed based on the Hartree-Fock approximation, but not restricted to a single Slater determinant trial space. The idea is to find a subspace of collective states which are strongly coupled to the ground state by providing a systematic technique to generate these basis states from a Hartree-Fock-like state. In the resulting basis space a residual diagonalization is easily performed. An application to a solvable model is made, both to justify and to investigate the structure of our approach.

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1. Introduction

In nuclear structure studies one is often interested only in the low-lying bound states. If a complete set of eigenstates is not needed, the large diagonalizations which occur in a shell model calculation may be avoided. This is the motivation for shape mixing calculations in deformed nuclei, where one mixes solutions of the Hartree-Fock (HF) equations which possess different deformation or shapes.

From a theoretical standpoint there is a clear motivation to base an approach on the variational principle: the many-body Schrödinger equation arises from it when the class of trial wave functions is unrestricted. The HF approximation [1] is obtained when the trial wave function is restricted to be a single Slater determinant (SD). If one also includes different configurations in the class of trial wave functions, then one obtains the multiconfiguration HF approach [2].

If a good description of the lowest-lying states of the system is desired, then one should know a priori which configurations should be included. Recently, Miller et al. [3–5] proposed a systematic approach for generating a set of basis states which are all solutions to the HF variational equations. Such an approach requires solving the HF problem not only once, but as many times as the number of basis states is desired.

The purpose of the present work is to propose a method, based on the variational principle, that constitutes a more efficient way of generating the basis states that precede a configuration mixing calculation. To achieve this goal, the HF problem is reformulated in a fashion that provides one with a novel way of viewing its inner structure.

Our formalism is presented in Sect. 2, while an application to a solvable model is discussed in Sect. 3. Some conclusions are drawn in Sect. 4.

2. Formalism

Our starting point is to consider the HF problem not from the customary (Roothaan's [1]) point of view but from a different perspective, by investigating the connection between the HF−SSD, $|\mathrm{HF}\rangle$, and a given "starting" SD, $|\Phi_0\rangle$, which usually (although by no means necessarily) will be the unperturbed ground state (u.g.s.)

$$|\Phi_0\rangle = \prod_{i=1}^{N} \alpha_i^\dagger |0\rangle. \tag{2.1}$$

This is the ground state (g.s.) of the N-fermion system when the Hamiltonian $\hat{H} = \hat{T} + \hat{V}$ reduces itself to its one-body part $\hat{T}$. According to Thouless [6], $|\Phi_0\rangle$ and $|\mathrm{HF}\rangle$ are related by

$$|\mathrm{HF}\rangle = \exp(i\hat{F})\,|\Phi_0\rangle \tag{2.2}$$

$\hat{F}$ being a hermitian one-body operator

$$\hat{F} = \sum_{\alpha\beta} f_{\alpha\beta}\, a_\alpha^\dagger a_\beta + \mathrm{H.C.}; \qquad \alpha \in |\Phi_0\rangle,\ \beta \notin |\Phi_0\rangle. \tag{2.3}$$

The HF problem can thus be regarded as that of determining $\hat{F}$: one is looking for that set of coefficients $f_{\alpha\beta}$ that (assuming $\langle\Phi_0|\Phi_0\rangle = 1$) minimizes

$$E_{\mathrm{HF}} = \langle\Phi_0|\exp(-i\hat{F})\hat{H}\exp(i\hat{F})\,|\Phi_0\rangle. \tag{2.4}$$

The variational principle leads then, immediately, to the HF equations, as shown for example in Ref. 6. But we could follow a different path by recourse to the commutation relationship between $\hat{H}$ and $\hat{F}$. Assuredly, this contains all the information that may be relevant for our purposes, since these two operators constitute the basic ingredients of the HF problem. Of course we do not know $\hat{F}$ (otherwise, there would be no problem to solve), but we may introduce a hierarchy of operators $\hat{C}_n$ given by

$$\hat{C}_0 = \hat{H} \tag{2.5}$$

$$\hat{C}_n = i[\hat{C}_{n-1}, \hat{F}], \qquad n = 1, 2, \ldots \tag{2.6}$$

whose $|\Phi_0\rangle$-expectation values are necessary for the evaluation of the HF energy, i.e.,

$$E_{\mathrm{HF}} = \sum_{n=0}^{\infty} \frac{1}{n!} \langle\Phi_0|\,\hat{C}_n\,|\Phi_0\rangle. \tag{2.7}$$

To calculate the $|\Phi_0\rangle$-expectation values of the $\hat{C}_n$, it is convenient to rewrite $\hat{H}$ in a somewhat more general fashion as

$$H \equiv C_0 = \sum_{ij} t_{ij}^{(0)} a_i^\dagger a_j + \tfrac{1}{4} \sum_{ikjl} V_{ijkl}^{(0)} a_i^\dagger a_j^\dagger a_l a_k \tag{2.8}$$

with

$$t_{ij}^{(0)} = t_{ij} \tag{2.9}$$

and

$$V_{ijkl}^{(0)} = V_{ijkl}, \tag{2.10}$$

denoting the matrix elements of the operators $\hat{T}$ and $\hat{V}$ respectively.

By construction, one can easily show that $\hat{C}_n$ is of the general form

$$\hat{C}_n = \sum_{ij} t_{ij}^{(n)} a_i^\dagger a_j + \tfrac{1}{4} \sum_{ijkl} V_{ijkl}^{(n)} a_i^\dagger a_j^\dagger a_l a_k \tag{2.11}$$

where $t_{ij}^{(n)}$ and $V_{ijkl}^{(n)}$ dependent both upon $t_{ij}^{(0)}$, $V_{ijkl}^{(0)}$ and on the $f_{\alpha\beta}$ that define $\hat{F}$. The set of relationships (2.6) leads now to recurrence relations for the matrix elements of (2.11), which in principle would solve our problem,

$$t_{ij}^{(n+1)} = i \sum_{\gamma \notin \Phi_0} \{t_{i\gamma}^{(n)} f_{j\gamma}^* - t_{\gamma j}^{(n)} f_{i\gamma}\} + i \sum_{\mu \in \phi_0} \{t_{i\mu}^{(n)} f_{\mu j} - t_{\mu j}^{(n)} f_{\mu i}^*\} \tag{2.12}$$

and

$$\begin{aligned} V_{ijkl}^{(n+1)} = i \sum_{\gamma \notin \phi_0} & \{f_{\gamma k}(V_{ij\gamma l}^{(n)} - V_{ijl\gamma}^{(n)}) + f_{\gamma i}(V_{j\gamma kl}^{(n)} - V_{\gamma jkl}^{(n)})\} \\ & + i \sum_{\mu \in \phi_0} \{f_{i\mu}(V_{j\mu kl}^{(n)} - V_{\mu jkl}^{(n)}) \\ & + f_{k\mu}^*(V_{ij\mu l}^{(n)} - V_{ijl\mu}^{(n)})\}. \end{aligned} \tag{2.13}$$

After a little algebra, one finds that the g.s. energy, in terms of the $t_{ij}^{(n)}$ and $V_{ijkl}^{(n)}$, adopts the appearance

$$E_{\mathrm{HF}} = \sum_{n=0}^{\infty} \frac{1}{n!} \{\sum_i t_{ii}^{(n)} + \tfrac{1}{4} \sum_{ij} (V_{ijij}^{(n)} - V_{ijji}^{(n)})\}. \tag{2.14}$$

Now, we can truncate the expansion of $\exp(i\hat{F})$ at order K, to obtain the K-th order of approximation of the HF g.s. energy,

$$E_K = \sum_{n=0}^{K} \frac{1}{n!} \{\sum_i t_{ii}^{(n)} + \tfrac{1}{4} \sum_{ij} (V_{ijij}^{(n)} - V_{ijji}^{(n)})\}. \tag{2.15}$$

For successive values of K, the parameters $f_{\alpha\beta}$ are determined by minimizing the approximate g.s. energy E given by (2.15). Suppose now that at order K, we obtain M different sets of parameters $f_{\alpha\beta}$. That set $\{f_{\alpha\beta}\}$ that yields the lowest value for E_K defines the K-th order approximation $|\mathrm{HF}\rangle$. But, if we also consider the other $(M-1)$ solutions, then we can determine a non-orthonormal, undercomplete basis given by

$$|\Psi_K^{(j)}\rangle = \exp(i\hat{F}_j)\,|\Phi_0\rangle: \qquad j = 1, \ldots, M, \tag{2.16}$$

where $\hat{F}_j$ is constructed with the j-th set $f_{\alpha\beta}$ which results from minimizing (2.15).

We are now in a position to perform, at each order of approximation K, a residual diagonalization of $\hat{H}$ within this undercomplete basis $|\Psi_K^{(j)}\rangle$ which leads to the following generalized eigenvalue problem

$$\sum_{j=1}^{M} H_{ij}^{(K)} d_j^{(K)} = E^{(K)} \sum_{j=1}^{M} \sigma_{ij}^{(K)} d_j^{(K)}, \qquad i = 1, \ldots, M, \tag{2.17}$$

where

$$H_{ij}^{(K)} = \langle\Psi_K^{(i)}|\,\hat{H}\,|\Psi_K^{(j)}\rangle, \tag{2.18}$$

and

$$\sigma_{ij}^{(K)} = \langle\Psi_K^{(i)}|\Psi_K^{(j)}\rangle, \tag{2.19}$$

detailed expressions being given in the Appendix.

The lowest eigenvalue of (2.17) will be our new approximation, at order K, for the exact g.s. energy. Even for small values of K one would expect good

results from these small diagonalization as this subspace is expected to include collective states which are strongly coupled to the g.s. Not *all* the M states one obtains from minimizing (2.15) should be included in this subspace: only those that correspond to small values of f are appropriate. In that situation, $|\Phi_0\rangle$ is not expected to differ too much from $|\mathrm{HF}\rangle$. The criterium by which one truncates this undercomplete basis will be discussed in the next Section.

3. Application to a Solvable Model

3.1. Description of the Model

We consider an exactly solvable model of the Lipkin type [7] proposed by Abecasis et al. [8, 9]. We deal with two N-fold degenerate single-particle (s.p.) levels, separated by the s.p. energy ε, and N identical fermions. Two quantum numbers characterize a given s.p. state. One of them adopt the values -1 (lower level) and $+1$ (upper level). The other, which may be called the "p-spin", singles out a state within the N-fold degeneracy. In order to write down the corresponding Hamiltonian we introduce the quasi-spin operators [7]

$$\hat{J}_+ = \hat{J}_-^\dagger = \sum_{p=1}^{N} a_{p+1}^\dagger a_{p-1}, \tag{3.1}$$

and

$$J_z = \tfrac{1}{2} \sum_{p=1}^{N} \sum_{\sigma=-1,1} \sigma a_{p\sigma}^\dagger a_{p\sigma}, \tag{3.2}$$

which fulfill SU(2) (angular momentum) commutation rules. With the energy given in units of the s.p. energy ε, the Hamiltonian reads [8, 9] (repulsive interaction)

$$\hat{H} = \hat{J}_z + \frac{V}{2}(\hat{J}^2 + \hat{J}_x - \hat{J}_x^2), \tag{3.3}$$

with

$$\hat{J}_x = \tfrac{1}{2}(\hat{J}_+ + \hat{J}_-) \tag{3.4}$$

$$\hat{J}^2 = \hat{J}_z^2 + \tfrac{1}{2}(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+). \tag{3.5}$$

$\hat{H}$ commutes with $\hat{J}^2$ and thus the exact solution is found by diagonalization within the g.s. multiplet with $J = N/2$ [9].

3.2. Application of our Formalism

Let us now apply to this model the formalism introduced in Sect. 2. We shall write the operator $\hat{C}_0$ of (2.8) in the following way:

$$\hat{C}_0 = \alpha_0 \hat{J}_z + \beta_0 \hat{J}_z^2 + \gamma_0 \hat{J}^2 + \delta_0 \hat{J}_+^2 + \delta_0^* \hat{J}_-^2 + \varepsilon_0 \hat{J}_+ + \varepsilon_0^* \hat{J}_-, \tag{3.6}$$

the constants α_0, β_0, γ_0, δ_0 and ε_0 being determined by comparison with the definition (3.3):

$$\begin{aligned} &\alpha_0 = 1, \\ &\beta_0 = \gamma_0 = \varepsilon_0 = V, \\ &\delta^0 = -\frac{V}{2}. \end{aligned} \tag{3.7}$$

Due to the fact that the interaction (3.3) does not depend explicitly upon the individual p-quantum numbers (all of them are equivalent), the arguments advanced by Agassi et al. [10] in order to construct the HF transformation for the Lipkin model will apply here as well. Consequently, the operator $\hat{F}$ adopts the extremely simple form (adopted in a different context by Mann & Gross [11])

$$\hat{F} = f\hat{J}_+ + f^* \hat{J}_-, \tag{3.8}$$

that is, $\hat{F}$ depends only upon one single (complex) parameter f. The next step is to find $\hat{C}_1$, and we obtain

$$\hat{C}_1 = i[\hat{C}_0, \hat{F}] = a_0 \hat{J}_+ + a_0^* \hat{J}_- + b_0(\hat{J}_+ \hat{J}_z + \hat{J}_z \hat{J}_+) + b_0^*(\hat{J}_- \hat{J}_z + \hat{J}_z \hat{J}_-) + c_0 \hat{J}_z \tag{3.9}$$

with

$$\begin{aligned} &a_0 = i\alpha_0 f, \\ &b_0 = i(\beta_0 f + 2\beta_0 f^*), \\ &c_0 = 2i(\varepsilon_0 f^* - \varepsilon_0^* f). \end{aligned} \tag{3.10}$$

The commutator of $\hat{C}_1$ and $\hat{F}$ gives

$$\hat{C}_2 = \alpha_1 \hat{J}_z + \beta_1 \hat{J}_z^2 + \gamma_1 \hat{J}^2 + \delta_1 \hat{J}_+^2 + \delta_1^* \hat{J}_-^2 + \varepsilon_1 \hat{J}_+ + \varepsilon_1^* \hat{J}_-, \tag{3.11}$$

with

$$\begin{aligned} &\alpha_1 = 2i(a_0 f^* - a_0^* f), \\ &\beta_1 = 6i(b_0 f^* - b_0^* f), \\ &\gamma_1 = -2i(b_0 f^* - b_0^* f), \\ &\delta_1 = 2b_0 f, \\ &\varepsilon_1 = c_0 f. \end{aligned} \tag{3.12}$$

Clearly, $\hat{C}_2$ has a structure identical to that of $\hat{C}_0$, which implies that $\hat{C}_1$ and $\hat{C}_3$ will also have the same structure, etc. The $\hat{C}_n$ are divided then into two groups, according to whether the subindex n is even or odd. Within each group, all operators have

identical structure, and one can write for the HF g.s. energy (2.7):

$$E_{\mathrm{HF}}=\sum_{n=0}^{\infty}\frac{1}{(2n)!}\langle ugs|\,\hat{C}_{2n}\,|ugs\rangle + \sum_{n=0}^{\infty}\frac{1}{(2n+1)!}\langle ugs|\,\hat{C}_{2n+1}\,|ugs\rangle. \tag{3.13}$$

Clearly, the recurrence relationships (2.12-2.13) translate themselves into the corresponding ones (3.10) and (3.12) which are easily solvable starting with (3.7). On account of the nature of the u.g.s. [7], we immediately find

$$\langle ugs|\,\hat{C}_{2n}\,|ugs\rangle=-\alpha_n J+\beta_n J^2+\gamma_n J(J+1) \tag{3.14}$$

and

$$\langle ugs|\,\hat{C}_{2n+1}\,|ugs\rangle=-c_n J, \tag{3.15}$$

so that, after introduction of these results into (3.13), we are led, by setting

$$x=2|f| \tag{3.16}$$

$$f=A+iB \tag{3.17}$$

to the result

$$E_{\mathrm{HF}}(A,B)=J\left\{V(N+1)-\cos(x)-2VB\frac{\sin(x)}{x} - VB^2(N-1)\frac{\sin^2(x)}{x^2}\right\}, \tag{3.18}$$

which is independent of the real part A of f. Minimization with respect to B leads to the desired HF solution. We do not need to pursue the subject any further in view of the fact that the expression to be minimized,

$$E_{\mathrm{HF}}=-J\cos(B)+VJ\{2J\cos^2(B)+\sin^2(B) +1+2\sin(B)\} \tag{3.19}$$

is the one obtained, following a totally different route, in Ref. 9. Thus, our formalism easily leads to the correct (previously known [9]) HF solution.

If we now keep a finite number of terms K in Eq. (3.13), we obtain our approximate expression for the HF energy. For simplicity we will only study those cases in which $K=2M$ (M integer). Our approximate energy E_K will be given by

$$E_K=-J\sum_{r=0}^{M}\frac{(-1)^r x^{2r}}{(2r)!}+\frac{VJ(2J-1)}{2}\sum_{r=0}^{M}\frac{(-1)^r(2x)^{2r}}{(2r)!} -\frac{VJ}{2}\sum_{r=0}^{M-1}\frac{(-1)^r x^{2r+1}}{(2r+1)!}+\frac{VJ(2J+3)}{2}, \tag{3.20}$$

Table 1. Approximate energies for the ground state, retaining the first K terms in (3.20). The second column shows the real values of x for which a minimum for the energy is obtained. The parameters of the model are $N=4$ and $V=1$

K	x	$E(x)$	K	x	$E(x)$
2	−0.4	8.757333	14	−0.420002	8.807252
4	−0.421999	8.808264		−2.800196	12.42967
	−1.034263	8.244145		1.445718	−0.124880
	1.195393	1.126105		−1.313649	7.747911
6	−0.419962	8.807235		3.149440	11.25360
8	−0.420002	8.807252	16	−0.420002	8.807252
	1.432947	−0.094270		−2.862564	12.5880
10	−0.420002	8.807252		−3.731462	9.681294
	−2.413473	10.61410		−1.313648	7.747912
	−1.314487	7.747259		1.445716	−0.124877
	2.603934	5.932571	18	−0.420002	8.807252
	1.445658	−0.124782		−2.853722	12.56816
12	−0.420002	8.807252		−1.313648	7.747912
	−1.313611	7.747937		3.406663	12.51426
	1.445658	−0.124782		1.445716	−0.124877

Table 2. The number of terms in (3.20) necessary to achieve a stable value for the ground state energy is shown as a function of the number of particles N and the product NV

N	N.V.	K	$E(K)$
4	0.4	8	−1.089048
20	0.4	8	−5.832454
40	0.4	8	−10.81802
4	2.0	16	−0.249008
40	2.0	16	−2.498999
4	4.0	20	−0.124877
40	4.0	20	−1.249877

E_K is clearly a polynomial of degree K in x, which should be minimized with respect to this variable. This procedure will lead to not one but *several* roots x_i, and we select, for obtaining the corresponding K-th order approximation to the HF energy, the one that gives the lowest E_K.

In Table 1 we list, for several values of K, the different E_K values that one obtains from the corresponding x_i (only the real ones are considered), for the case $N=4$ and $V=1$. We need 14 terms in (3.20) in order to achieve convergence within four significant digits. The number of terms needed in Eq. (3.20) in order to obtain a stable energy value depends on the product NV. Some examples are shown in Table 2. The "convergence" of (3.20) is by no means a rapid one, although the number of terms required can be considered a manageable one.

Now, the "leit-motiv" of this work is that of investigating the possibility of obtaining better approximations to the exact ground state energy than E_{HF}, by diagonalizing $\hat{H}$ in the non-orthonormal

Table 3. Ground state energies for different coupling constants V (expressed in terms of $V_c=0.0333$) for $N=16$

V	0.6	0.9	1.0	1.1	1.4
Exact energy	−5.329	−4.094	−3.729	−3.404	2.678
E(Hartree-Fock)	−5.296	−4.023	−3.662	−3.351	−2.655
E(present approach)	−5.323	−4.074	−3.887	−3.376	−2.655
K	6	28	28	28	28
Diagonalization order	2×2	5×5	5×5	5×5	7×7

undercomplete basis generated by our algorithm. We proceed now in this direction.

In view of the simplicity of the model, things work out here in a very simple fashion. No matter how large K may be, the number of real roots x_i of (3.20) is never larger. As a matter of fact, it does not, in any circumstance, exceed the value $K=7$. Some typical results are displayed in Table 3 for $N=16$. The exact ground state energy is obtained by means of a 17×17-matrix diagonalization. With our method, just a 2×2 or, at most, a 7×7 one gives already satisfactory figures. The coupling constants are given in terms of the Mann and Gross "critical" one: $V_c=0.0333$ (for $N=16$) [11, 12]. The Hartree-Fock energy E_{HF} is also given (which, due to the peculiarities of these "Lipkin-like" models, constitutes always a good approximation [2, 9, 10]. The results of the diagonalization within the present scheme are given, together with both the value of K employed and the order of the corresponding matrix.

4. Conclusions

The HF approach has been reformulated in a novel way by recourse to the Thouless representation of the HF Slater determinant. The HF problem is here regarded as that of determining the one-body operator $\hat{F}$ of Eq. (2.2), and the corresponding problem is tackled by studying the commutation relations between $\hat{H}$ and $\hat{F}$. A hierarchy of operators $\hat{C}$ arises from this study, that allows for a compact expression for the HF energy (Eqs. (2.7) and (2.14)). The latter has a vivid "perturbative" appearance, and its truncation leads, in a natural fashion, to different approximations to E_{HF}. These, however, do not constitute the "leit-motiv" of this work. It is rather the fact that, after truncation of (2.14) to order K (cf. Eq. (2.15)), the minimization procedure for E_K yields several solutions. To each of them corresponds a different SD, and these form an undercomplete basis that arises out of a process where the dynamics of the problem plays clearly a dominant role. Diagonalizing $\hat{H}$ in this basis generates then a "dynamically-motivated" algorithm, based upon the variational principle. Applications to an exactly solvable model (Sect. 4) illustrate the power of the proposed approach.

Appendix

For the sake of completeness we now derive the matrix elements of the Hamiltonian $\hat{H}$ in the residual subspaces.

The states $|\Psi_K^{(j)}\rangle$ (see Eq. (2.16)) admit the following expansion:

$$|\Psi_K^{(j)}\rangle=\sum_{n=0}^{K}\frac{(if_j)^n}{n!}|0\rangle=\sum_{l=0}^{N/2}C_{K,2l}^{(j)}|2l\rangle + \sum_{n=0}^{N/2-1}C_{K,2l+1}^{(j)}|2l+1\rangle, \tag{A.1}$$

where $|l\rangle$ denotes the configuration in which l particles are in the upper level and $N-l$ in the lower level. The coefficients $C_{K,l}^{(j)}$ are easily obtained from the following recurrence relations:

$$C_{K,2l}^{(j)}=\sum_{n=0}^{M}\frac{(-x_j)^{2n}}{(2n)!}C_{2l}^{(2n)},$$
$$C_{K,2l+1}^{(j)}=\sum_{n=0}^{M-1}\frac{(-x_j)^{2n+1}}{(2n+1)!}C_{2l+1}^{(2n+1)}, \tag{A.2}$$

with

$$C_0^{(2n+2)}=(2N(N-1))^{1/2}C_2^{(2n)}-NC_0^{(2n)}\quad n=0,\ldots,M-1$$
$$C_1^{(2n+3)}=(6(N-1)(N-2))^{1/2}C_3^{(2n+1)}+(2-3N)C_1^{(2n+1)}\quad n=0,\ldots,M-2$$
$$C_{2i}^{(2n+2)}=[(2i+1)(2i+2)(N-2i)(N-2i-1)]^{1/2}C_{2i+2}^{(2n)}-[2i(N-2i+1)+(2i+1)(N-2i)]C_{2i}^{(2n)}+[2i(2i-1)(N-i+1)(N-2i+2)]^{1/2}C_{2i-2}^{(2n)}$$
$$i=1,\ldots,\frac{N}{2}-1;\quad n=0,\ldots,M-1$$

$$C_{2i+1}^{(2n+3)}$$
$$= [2i(2i+1)(N-2i)(N-2i+1)]^{1/2} C_{2i-1}^{(2n+1)}$$
$$- [(N-2i-1)(2i+2)+(2i+1)(N-2i)] C_{2i+1}^{(2n+1)}$$
$$+ [2(i+1)(2i+3)(N-2i-1)(N-2i-2)]^{1/2} C_{2i+3}^{(2n+1)}$$
$$n=0, \ldots, M=2; \quad i=0, \ldots, M=2 \tag{A.3}$$

$$C_{N-1}^{(2n+3)} = (6(n-1)(N-2))^{1/2} - (3N-2) C_{N-1}^{(2n+1)}$$
$$n=0, \ldots, M-2$$

$$C_{N}^{(2n+2)} = (2N(N-1))^{1/2} C_{N-2}^{(2n)} - N C_{N}^{(2n)}$$
$$n=0, \ldots, M-1$$

with the initial values

$$C_0^{(0)} = 1,$$
$$C_1^{(1)} = \sqrt{N}. \tag{A.4}$$

Finally, the matrix elements needed for the residual diagonalization (2.17-2.19) are given by

$$\sigma_{ij}^{(K)} = \sum_{l=0}^{J} C_{K,2l}^{(i)} C_{K,2l}^{(j)} + \sum_{l=0}^{J-1} C_{K,2l+1}^{(i)} C_{K,2l+1}^{(j)} \tag{A.5}$$

and

$$\begin{aligned} {}^{(K)}_{ij} = & \sum_{l=0}^{J} \sum_{l'=0}^{J} C_{K,2l}^{(i)} C_{K,2l'}^{(j)} \langle 2l | H | 2l' \rangle \\ & + \sum_{l=0}^{J-1} \sum_{l'=0}^{J-1} C_{K,2l+1}^{(i)} C_{K,2l'+1}^{(j)} \langle 2l+1 | H | 2l'+1 \rangle \\ & + \sum_{l=0}^{J-1} \sum_{l'=0}^{J} (C_{K,2l+1}^{(i)} C_{K,2l'}^{(j)} \\ & + C_{K,2l'+1}^{(i)} C_{K,2l}^{(j)} \langle 2l | H | 2l'+1 \rangle \end{aligned} \tag{A.6}$$

where the matrix elements $\langle l | H | l' \rangle$ are given in Ref. 9.

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