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Reduced Hamiltonians.
I: Spin-adapted and spin-nonadapted reduced Hamiltonians

Josep Planelles [1]

Department of Applied Mathematics, University of Waterloo, Waterloo,
Ontario, Canada N2L 3G1

Pascual Viciano

Departament de Ciències Experimentals, Universitat Jaume I, Apartat 224,
12080 Castelló, Spain

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Closed formulae are derived for matrix elements of spin-nonadapted reduced Hamiltonians in a finite-dimensional, antisymmetric Hilbert space. The role of the spin-adaptation is discussed. Some numerical results confirm that this role is not critical for approaches based upon the eigenvectors of these Hamiltonians.

1. Introduction

The reduction of an N-electron problem to an effective two-electron one has been of great interest for many years. We cannot provide here specific details of these developments and refer instead the interested reader to original papers [1–18]. These developments can be roughly divided into two groups: (i) those in which the reduction procedure is applied to the wavefunction, yielding density matrices [4–14], and (ii) those, in which the reduction is applied to the Hamiltonian [16–28].

In general, the efforts to formulate an N-electron theory in terms of reduced density matrices, while employing the variational principle, bear heavily on the N-representability problem (see, e.g., [29]). In contrast, the reduced Hamiltonian approach is a non-variational procedure that effectively describes an N-electron system by a reduced Hamiltonian acting in a p-body space ($p<N$). The main emphasis in this approach is on the eigenfunctions of the Hamiltonian. This

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[1] Permanent address: Departament de Ciències Experimentals, Universitat Jaume I, Apartat 224, 12080 Castelló, Spain.

approach was employed by several authors [17,18,23] but the obtained results have not fulfilled the expectations that were initially associated with it.

Another method employing the idea of reduced Hamiltonians was formulated by Valdemoro [24–26]. Her approach is closer to the reduced density matrix formalism and employs the contraction mapping relating reduced density matrices of different order [13,14,24–26] to define the required reduced Hamiltonians. In essence, these Hamiltonians are obtained by applying a contraction mapping to an N-electron Hamiltonian defined in a spin-adapted and antisymmetric full configuration interaction (FCI) Hilbert space. The resulting reduced Hamiltonian depends on the total number of electrons, N, the total spin, S, and the number of orbitals, K, associated with the FCI Hilbert space in which the original N-electron Hamiltonian is defined. This spin-adapted reduced Hamiltonian (SRH), is N- and S-representable [8] by construction. It should be stressed that the spin adaptation of the Hamiltonian is independent of the reduction mapping. So far, two different spin projections were employed [25,26]: projection upon S^2 and S_z eigenspaces and projection upon only S_z adapted spaces. However, no attempt has yet been made to employ spin non-adapted reduced Hamiltonians (RH).

It is the aim of this paper to present general expressions for spin-nonadapted RH matrix elements. These are much simpler than those for the SRH, and the eigenvectors of both operators are generally different when finite-dimensional Hilbert spaces are employed. However, these eigenvectors are identical in the limit of complete (either spin-adapted or spin-nonadapted) infinite-dimensional Hilbert spaces.

The paper is organized as follows. In section 2 we give a survey of previous theoretical results. In particular, we emphasize that the spin-adaptation influences only the coefficients at the integrals that appear in the expression for the reduced Hamiltonian. Consequently the spin-adaptation can be performed independently of the contraction itself. In section 3, the general formulation of the RH is given and, finally, in section 4 we present the asymptotic behavior of the eigenvectors of both reduced Hamiltonians in complete Hilbert spaces and discuss the role of spin-adaptation. Some numerical results from the one-body spin-adapted and spin-nonadapted reduced Hamiltonians are presented to provide an additional insight.

2. Survey of previous results

Density matrices of different order are related as follows [13,24–26]:

$$ {}^{p}D^{\mathcal{L}}_{\xi\theta} = \frac{\binom{N}{p}}{\binom{N}{q}\binom{q}{p}} \sum_{\Xi,\Theta} {}^{p}D^{\Xi\Theta}_{\xi\theta}\, {}^{q}D^{\mathcal{L}}_{\Xi\Theta} \,, \tag{1} $$

where $|\Xi\rangle, |\Theta\rangle$ and $|\xi\rangle, |\theta\rangle$ are q-electron and p-electron configurations, respectively; ${}^{p}D^{\mathcal{L}}$ and ${}^{q}D^{\mathcal{L}}$ are p- and q-reduced density matrices corresponding to the N-electron wave function $|\mathcal{L}\rangle$; and ${}^{p}D^{\Xi\Theta}$ is the pth order $\Xi\Theta$-transition density matrix. The reducing mapping (1) results as a natural consequence of the commutation properties of fermion creation and annihilation operators of the second quantization formalism [25,26].

Let us recall that the spectral decomposition of an N-electron Hamiltonian $\mathbb{H}$ takes the form

$$\mathbb{H} = \sum_{\mathcal{L}} E_{\mathcal{L}} |\mathcal{L}\rangle\langle\mathcal{L}| = \sum_{\mathcal{L}} E_{\mathcal{L}} \mathcal{D}^{\mathcal{L}} , \tag{2}$$

where $\mathrm{E}_{\mathcal{L}}$ is the exact eigenvalue that would be obtained by an FCI calculation, $|\mathcal{L}\rangle$ is the corresponding eigenvector and $\mathcal{D}^{\mathcal{L}}$ represents the N-body non-reduced density matrix. If we close eq. (2) by the N-electron configurations $|\Lambda\rangle$ and $|\Omega\rangle$, we get the corresponding matrix element,

$$\mathbb{H}_{\Lambda\Omega} = \sum_{\mathcal{L}} E_{\mathcal{L}} \mathcal{D}^{\mathcal{L}}_{\Lambda\Omega} . \tag{2'}$$

If we now multiply both sides of eq. (2′) by ${}^{p}\mathrm{D}^{\Lambda\Omega}_{\lambda\gamma}$ (the λ, γ element of the p-body $\Lambda\Omega$-transition matrix) and sum over all Λ, Ω, we obtain

$$\sum_{\Lambda\Omega} \mathbb{H}_{\Lambda\Omega} {}^{p}D^{\Lambda\Omega}_{\lambda\gamma} = \sum_{\mathcal{L}} E_{\mathcal{L}} \sum_{\Lambda\Omega} \mathcal{D}^{\mathcal{L}}_{\Lambda\Omega} {}^{p}D^{\Lambda\Omega}_{\lambda\gamma} = \sum_{\mathcal{L}} E_{\mathcal{L}} {}^{p}D^{\mathcal{L}}_{\lambda\gamma} , \tag{3}$$

the last equality resulting from eq. (1) (note that in this case $q = N$). Equation (3) now implies the definition of the reduced Hamiltonian, namely

$${}^{p}H'_{\lambda\gamma} = \sum_{\Lambda\Omega} \mathbb{H}_{\Lambda\Omega} {}^{p}D^{\Lambda\Omega}_{\lambda\gamma} = \sum_{\mathcal{L}} E_{\mathcal{L}} {}^{p}D^{\mathcal{L}}_{\lambda\gamma} . \tag{4}$$

It must be stressed that while eq. (2′) represents the spectral decomposition of the FCI Hamiltonian, eq. (4) does not, since the reduced density matrices are not orthogonal.

Now, the N-electron Hamiltonian may be written in the form [27,30]

$$\hat{H} = \frac{1}{2} \sum_{ijkl} \{ij|kl\} \, {}^{2}E^{ik}_{jl} , \tag{5}$$

where

$$\{ij|kl\} = \langle i(1)|\langle k(2)|\hat{h}_2(1,2)|l(2)\rangle|j(1)\rangle + \frac{1}{N-1} [\delta_{kl} \langle i(1)|\hat{h}_1(1)|j(1)\rangle + \delta_{ij} \langle k(1)|\hat{h}_1(1)|l(1)\rangle] \tag{6}$$

are the generalized two-electron integrals, and ${}^{2}E^{ik}_{jl}$ are spin-free density operators [31] related to density matrices:

$${}^{2}D^{\Lambda\Omega}_{ij;kl} = \frac{1}{2!} \langle\Lambda| \, {}^{2}E^{ik}_{jl} |\Omega\rangle . \tag{7}$$

Finally, by substituting Hamiltonian (5) into eq. (4), using the definition of the unit operator $\mathbb{1} = \sum |\Omega\rangle\langle\Omega|$, and the notation

$$ {}^pD^{\Lambda\Omega}_{\lambda,\gamma} = \frac{1}{p!}\langle\Lambda|{}^pE^{\lambda}_{\gamma}|\Omega\rangle \,, \tag{7'} $$

where λ and γ are strings or orbital labels, we get

$$ \begin{aligned} {}^pH'_{\lambda\gamma} &= \sum_{\Lambda\Omega}\tfrac{1}{2}\sum_{ijkl}\{ij|kl\}\langle\Lambda|{}^2E^{ik}_{jl}|\Omega\rangle\frac{1}{p!}\langle\Lambda|{}^pE^{\lambda}_{\gamma}|\Omega\rangle \\ &= \frac{1}{2}\frac{1}{p!}\sum_{ijkl}\{ij|kl\}\sum_{\Omega}\langle\Omega|{}^2E^{ik}_{jl}\left(\sum_{\Lambda}|\Lambda\rangle\langle\Lambda|\right){}^pE^{\lambda}_{\gamma}|\Omega\rangle \\ &= \frac{1}{2}\frac{1}{p!}\sum_{ijkl}\{ij|kl\}\langle\langle{}^2E^{ik}_{jl}\,{}^pE^{\lambda}_{\gamma}\rangle\rangle \,. \end{aligned} \tag{8} $$

The last equality uses the notation $<< \ >>$ to denote the trace.

We would like to stress the fact that if $|\Lambda\rangle$ and $|\Omega\rangle$ represent spin-adapted N-electron configurations, the trace in eq. (8) runs over N-electron configurations that are eigenfunctions of the spin operators $\widehat{S^2}$ and $\widehat{S}_z$ with eigenvalues S and M. This means that the sum runs over a basis of an antisymmetric component of a spin-adapted Hilbert space

$$ H^A(N,K,S,M) = (V_{2K}^{\otimes N})^A_{SM} \,, \tag{9} $$

where the superscript A indicates the antisymmetric component and the spin quantum numbers S, M label the eigenvalues of spin operators. The one-electron space V_{2K} is spanned by a set of $2K$ spin-orbitals, and is a product of the K-dimensional orbital space,

$$ V_K = \operatorname{span}\{\phi_k\}_{k=1}^{K} \,, \tag{10} $$

spanned by a set of K orthonormal orbitals, and the two-dimensional spin space.

On the other hand, if $|\Lambda\rangle$ and $|\Omega\rangle$ represent Slater determinants, the trace in eq. (8) runs over a basis of the Hilbert space $H^A(N,K)$,

$$ H^A(N,K) = (V_{2K}^{\otimes N})^A \,, \tag{11} $$

an antisymmetric component of the N-fold tensorial product of a one-electron space.

Thus, the general structure of the SRH and the RH is formally identical, and is given by eq. (8), the only difference being the space in which the traces are calculated.

3. Matrix elements of reduced Hamiltonians

Equation (8) may be further simplified by taking into account several symmetry relations that are satisfied by generalized two-electron integrals and by traces of products of density operators. A comprehensive study of matrix elements of SRHs was already carried out by one of us [28]. This study showed that the traces in eq. (8) may be classified into the following three types:

$$\text{(a)}\quad \alpha = \langle\langle {}^2E^{ab}_{qr}\,{}^pE^{qrs\ldots}_{abc\ldots}\rangle\rangle\,,$$

with $\{q,r\} \neq \{a,b\}$ while, as a whole, $\{a,b,q,r,s\ldots\} = \{q,r,a,b,c\ldots\}$.

$$\text{(b)}\quad \beta = \langle\langle {}^2E^{ka}_{\hat{T}(kq)}\,{}^pE^{qrs\ldots}_{abc\ldots}\rangle\rangle\,,$$

with $a \neq q$ and $\hat{T}$ a permutation of the S_2 group (i.e., the identity or a transposition), and

$$\text{(c)}\quad \mu = \langle\langle {}^2E^{kl}_{\hat{T}(kl)}\,{}^pE^{qrs\ldots}_{abc\ldots}\rangle\rangle\,.$$

Several distinct cases for each type must be considered, and this number increases with the increasing order p of the p-SRH. For example, there are four independent β-coefficients, four independent μ-coefficients and two independent α-coefficients in 2-SRH. The 3-SRH has four α-, eight β- and six μ-coefficients. The total number of independent coefficients of the 4-SRH is 34, etc.

Since the difference between the SRH and the RH coefficients is only in the space in which these traces are calculated, it would seem, on the first sight, that both matrices have the same number of coefficients. However, there exist certain symmetry relationships between these coefficients when calculated in the larger, spin-nonadapted space, so that irrespective of the order p of the p-RH, there is only one independent coefficient of each kind. From a practical point of view, we choose for this coefficient the one having a maximum coincidence of upper and lower indices, namely

$$\begin{aligned}
\alpha &= \langle\langle {}^2E^{ab}_{qr}\,{}^pE^{qrcde\ldots}_{abcde\ldots}\rangle\rangle = \langle\langle {}^2E^{12}_{34}\,{}^pE^{3456\ldots(p+2)}_{1256\ldots(p+2)}\rangle\rangle\,,\\
\beta &= \langle\langle {}^2E^{ka}_{kq}\,{}^pE^{qbcde\ldots}_{abcde\ldots}\rangle\rangle = \langle\langle {}^2E^{12}_{13}\,{}^pE^{3456\ldots(p+2)}_{2456\ldots(p+2)}\rangle\rangle\,,\\
\mu &= \langle\langle {}^2E^{kl}_{kl}\,{}^pE^{abcde\ldots}_{abcde\ldots}\rangle\rangle = \langle\langle {}^2E^{12}_{12}\,{}^pE^{3456\ldots(p+2)}_{3456\ldots(p+2)}\rangle\rangle\,.
\end{aligned} \tag{12}$$

Since traces are independent of the numbering of orbitals employed, we can use the expressions on the right-most sides of eq. (12), where specific orbitals are used.

The additional coefficients arising in the p-RH are then related to those given above, eq. (12), by appropriate permutations of labels of the two- and p-body density operators. We designate these coefficients as $\alpha(Q)$, $\beta(Q)$ and $\mu(Q)$, and the generic ones by $C(Q)$, where Q stands for a particular permutation ($Q \in S_2 \otimes S_p$) yielding the desired coefficient when acting on the corresponding standard coefficient defined by eq. (12). The next simple formula related a general $C(Q)$ coefficient with the corresponding standard one, designated by C, so that

$$C(Q) = (-\tfrac{1}{2})^q C\,, \tag{13}$$

where q is related to the permutation Q.

If the cycle structure of Q is $Q = 1^{a_1} 2^{a_2} \dots r^{a_r}$, then q is given by

$$q = \sum_{j=2}^{r} (j-1) a_j\,. \tag{14}$$

The proof of eq. (13) is given in appendix A.

A great simplification of coefficients (12) leads to a much simpler structure of matrix elements of the RH vs. the SRH. For example, in the less favourable case of a two-body Hamiltonian (note that as the order of the Hamiltonian increases, the ratio (number of RH-coefficients/number of SRH-coefficients) decreases, the formula yielding a general 2-SRH matrix element is

$$\begin{aligned}(\text{2-SRH})^{pq}_{rs} = {} & A_1\{pr|qs\} \\ & + A_2\{ps|qr\} \\ & + B_1[\delta_{pr}\{qs|aa\} + \delta_{qs}\{pr|aa\}] \\ & + C_1[\delta_{pr}\{qa|as\} + \delta_{qs}\{pa|ar\}] \\ & + B_2[\delta_{ps}\{qr|aa\} + \delta_{qr}\{ps|aa\}] \\ & + C_2[\delta_{ps}\{qa|ar\} + \delta_{qr}\{pa|as\}] \\ & + F_1\delta_{pr}\delta_{qs}\{aa|a'a'\} \\ & + G_1\delta_{pr}\delta_{qs}\{aa'|a'a\} \\ & + F_2\delta_{ps}\delta_{qr}\{aa|a'a'\} \\ & + G_2\delta_{ps}\delta_{qr}\{aa'|a'a\}\,. \end{aligned} \tag{15}$$

Equation (15) collects in a unique formula all possible cases of matrix elements given previously (eqs. (78)–(84) in [27]). Here the notation has been simplified and the expression written in a more symmetric way, having compacted it as much as possible. Nevertheless, the expression is still complex in view of the complexity of the SRH structure. The notation used here is the same as in the previous paper on general p-SRH matrix elements [28]. In eq. (15), A_1, A_2 are α-coefficients, B_1, B_2, C_1, C_2 are β-coefficients and F_1, F_2, G_1, G_2 are μ-coefficients; $\{pq|rs\}$ designate generalized two-electron integrals (see eq. (6)) and

$$
\begin{aligned}
\{qs|aa\} &= \sum_{k}^{K} \{qs|kk\}\,, \\
\{qa|as\} &= \sum_{k}^{K} \{qk|ks\}\,, \\
\{aa|d'd'\} &= \frac{1}{2}\sum_{kl}^{K} \{kk|ll\}\,, \\
\{ad'|d'a\} &= \frac{1}{2}\sum_{kl}^{K} \{kl|lk\}\,. \qquad (16)
\end{aligned}
$$

In contrast, a general matrix element formula for the 2-RH is,

$$
\begin{aligned}
(\text{2-RH})^{pq}_{rs} =& \alpha[pr|qs] + \sum_{T}^{\mathrm{S}_2} (-\tfrac{1}{2})^t \hat{T}(rs)\{\beta(\delta_{pr}[qs|aa] \\
&+ \delta_{qs}[pr|aa]) + \mu\delta_{pr}\delta_{qs}[aa|d'd']\}\,, \qquad (17)
\end{aligned}
$$

where $[pr|qs] = \{pr|qs\} - \frac{1}{2}\{ps|qr\}$, the permutation $\hat{T}(rs)$ may be either, the identity or the transposition (rs), and t is the parity of $\hat{T}$.

A comparison of eqs. (15) and (17) gives us an idea about the different complexity of the SRH and the RH. This different complexity, which reflects the differences between the $H^A(N, K, S, M)$ and the $H^A(N, K)$ Hilbert spaces, is most evident when calculating coefficients in practical cases. There are no closed formulas for these coefficients when considering $H^A(N, K, S, M)$ and a procedure involving characters of the irreducible representations of the symmetric group S_{p+2} (p is the order of the SRH) must be used. The complexity of this procedure rises very fast with p, since the symmetric group is involved [32]. In contrast, we have three very simple closed formulas, namely eqs. (12), for these coefficients when considering $H^A(N, K)$. The explicit formulas for these coefficients are derived in appendix B.

4. Asymptotic behaviour in complete Hilbert spaces. The role of spin-adaptation

It has been stated [25,26,33] that the role of the spin-adaptation in the SRH approach is to incorporate, in the reduced Hamiltonian, the information about the spin-symmetry of the N-electron system. On the other hand, as pointed out in section 1, the eigenvectors are the most useful objects yielded by the reduced Hamiltonians. In particular, within the SRH framework, several procedures of building approximate density matrices from the eigenvectors of the SRH have been proposed [26,34]. In order to discuss the role of the spin adaptation of reduced Hamiltonians, we display the coordinate representation of a properly renormalized, spin-adapted, two-body reduced Hamiltonian $\tilde{H}'$ (1, 2), defined in an asymptotically complete infinite-dimensional Hilbert space [35],

$$\begin{aligned}\tilde{H}'(1,2) &= 2(a^+ + 3a^-)\hat{H}(1,2) + (3\omega^+ + 3\omega^-) \\ &= k_1\hat{H}(1,2) + k_2 .\end{aligned} \tag{18}$$

Here $\hat{H}(1,2) = \hat{h}_1(1) + \hat{h}_1(2) + \hat{h}_2(1,2)$ and $a^+, a^-, \omega^+, \omega^-$ are constants depending on the number of electrons N, the spin-symmetry and some other magnitudes related to a statistical description of the N-electron Hamiltonian spectrum [35]. Then k_1 and k_2 are constants.

It is obvious from eq. (18) that $\tilde{H}'(1,2)$ and $\hat{H}(1,2)$ have the same eigenvectors and their eigenvalues are simply related. The k_1 and k_2 constants imply a scaling and a shift yielding the eigenvalues of $\tilde{H}'(1,2)$ from those of $\hat{H}(1,2)$. Since these constants depend upon the spin-symmetry of the N-electron system, the scaling will be different for each spin-symmetry of the N-electron system.

We can thus conclude that in the asymptotic case of complete Hilbert spaces, the eigenvectors of differently spin-adapted reduced Hamiltonians are the same and thus identical to those associated with the spin-nonadapted RH. However, the spin-adaptation distinguishes the corresponding eigenvalues. All these reasonings would seem to indicate that the spin-adaptation is important for approaches that are based on the eigenvalues of the SRH. However, it is not clear what is the role of spin-adaptation in the approaches based on eigenvectors. When we deal with finite-dimensional model spaces, the eigenvectors of the SRH and the RH are not the same, but approach one another when the space is being completed. The role, if any, that we could assign to the spin-adaptation in finite-dimensional model spaces may thus be related to the different dimensionality of the spin-adapted N-electron Hilbert spaces. The dimension of this space, built from a K-dimensional orbital space, is given by the Weyl–Paldus formula [36],

$$D(N,K,S) = \frac{2S+1}{K+1}\begin{bmatrix} K+1 \\ \frac{1}{2}N - S\end{bmatrix}\begin{bmatrix} K+1 \\ \frac{1}{2}N + S + 1\end{bmatrix} . \tag{19}$$

In order to give some insight into the role of spin-adaptation in approaches based upon the eigenvectors of reduced Hamiltonians, we include a set of calculations on spin-adapted and spin-nonadapted one-body reduced Hamiltonians (1-SRH and 1-RH), considering the ground state of atoms in the first row of the periodic system. The calculations were performed in a DZ basis set [37]. This basis set is not an ideal one for a configuration interaction calculation and the description of excited states, but it is very convenient from a computational point of view. It is also designed for the study of ground states and thus convenient for our purposes.

For each of the studied atoms, we obtained the eigenvectors of the one-body spin-nonadapted reduced Hamiltonian, 1-RH, and those of the 1-SRH (this Hamiltonian was adapted to the spin symmetry of the ground state of the studied atom). The independent quasiparticle, IQP, method [26] assumes that these vectors are

Table 1
Performance of the eigenvectors of RH and SRH as natural orbitals for the ground state of the first row elements. The expression for the coefficient ϵ is given in eq. (24).

Atom	ϵ_{IQP}	
	RH	SRH
Li	0.003	0.003
Be	0.005	0.005
B	0.058	0.048
C	0.029	0.028
N	0.014	0.014
O	0.007	0.006
F	0.002	0.002
Ne	0.002	0.002

approximate natural orbitals for all the states of the system. On the other hand, the best approximate natural orbitals for the ground state in an independent particle model are the eigenvectors of a self-consistent (SCF) calculation. We thus compare the ground state natural orbitals of the 1-SRH and the 1-RH with the SCF orbitals. As a parameter of comparison we choose the coefficient

$$\epsilon_{\text{IQP}}^{X} = \frac{1}{N}\left(N - \sum_{i}^{\text{occ}} \langle \phi_i^{\text{SCF}} | \psi_{i,X}^{\text{IQP}} \rangle\right), \tag{20}$$

where N is the number of electrons and X is either the RH or the SRH. We expect the best IQP method to approximate the variational independent particle (SCF) model. The results are shown in table 1. From this table we can conclude that the spin-adaptation does not essentially improve the quality of the vectors that are used in the construction of density matrices.

On the other hand, it was established [34] that we can get better density matrices when using eigenvectors of higher order p-SRH. Of course, the computational programs needed to built such p-SRH are more complex. Taking into account that the role of spin-adaptation is not decisive, it would be more economical to use much simpler RHs rather than SRHs.

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Appendix A

Proof of eq. (13)

First, we are going to prove eq. (13) for the case of μ-type coefficients, and subsequently, will generalize it to other cases.

The coefficient μ, eq. (12), may be written as $\langle\langle {}^{p+2}E^{123456\ldots(p+2)}_{123456\ldots(p+2)}\rangle\rangle$. An arbitrary μ-type coefficient, denoted as $\mu(Q)$, is then written as

$$\mu(Q) = \langle\langle {}^{p+2}E^{Q(123456\ldots)}_{123456\ldots}\rangle\rangle . \tag{A.1}$$

Let Q be a general permutation with the cycle structure $1^{a_1}2^{a_2}\ldots r^{a_r}$. The cycles of Q act as independent operators because no label can belong to more than one cycle. We can thus assume that Q is an r-cycle. The independence of cycles enables a straightforward generalization to an arbitrary Q.

Let us write $\mu(Q)$ in terms of fermion operators of the second quantization formalism [31,32],

$$\begin{aligned}\mu(Q) &= \left\langle\left\langle \sum_{\sigma_1\sigma_2\sigma_3\ldots} B^{Q(123456\ldots)}_{\sigma_1\sigma_2\sigma_3\ldots}\ {}^{+}B^{123456\ldots}_{\sigma_1\sigma_2\sigma_3\ldots}\right\rangle\right\rangle \\ &= (-1)^q\left\langle\left\langle \sum_{\sigma_1\sigma_2\sigma_3\ldots} B^{123456\ldots}_{Q(\sigma_1\sigma_2\sigma_3\ldots)}\ {}^{+}B^{123456\ldots}_{\sigma_1\sigma_2\sigma_3\ldots}\right\rangle\right\rangle .\end{aligned} \tag{A.2}$$

The averages involved in the trace vanish unless both strings of spin labels, corresponding to the creation and the annihilation operators, are identical. Consider thus, those r labels that are affected by the permutation (the remaining non-permuted labels may thus be ignored).

The summation over σ_i extend over two distinct spin orientations α and β. For the r labels considered we have 2^r possible orderings. The only strings that are invariants under Q are those involving the same spin everywhere, i.e., $\alpha_1\alpha_2\alpha_3\alpha_4\ldots$ and $\beta_1\beta_2\beta_3\beta_4\ldots$. Thus, amongst all these 2^r terms of $\mu(Q)$ only two give nonzero contribution to the trace. On the other hand, every contribution yields the same mean value. As a consequence, the $\mu(Q)$ coefficient is $(1/2)^{r-1}$ smaller than μ, what proves eq. (13) for this type of coefficients.

Let us next consider the case of β-coefficients (we omit the proof for the α-type coefficients, since it follows exactly the same lines as the proof for the β-type coefficients). Since $Q \in S_2 \otimes S_p$, we may write an arbitrary $\beta(Q)$ coefficient as

$$\beta(Q) = \langle\langle {}^{2}E^{P(12)}_{13}\, {}^{p}E^{R(3456\ldots)}_{2456\ldots}\rangle\rangle , \tag{A.3}$$

where $Q = PR = RP$. Applying the generalized Wick theorem, we find that

$$\begin{aligned}\beta(Q) &= \langle\langle {}^{p+2}E^{PR(123456\ldots)}_{132456\ldots}\rangle\rangle + \langle\langle {}^{p+1}E^{P(12)456\ldots)}_{1R^{-1}(2456\ldots)}\rangle\rangle \\ &= \langle\langle {}^{p+2}E^{Q(123456\ldots)}_{132456\ldots}\rangle\rangle + \langle\langle {}^{p+1}E^{Q(12456\ldots)}_{12456\ldots}\rangle\rangle .\end{aligned} \tag{A.4}$$

Each term in eq. (A.4) may be regarded as a μ-type coefficient. Thus, Q produces the same scalar factor in both terms on the right-hand side of eq. (A.4), and this factor was found to be given, for the μ-type coefficients, by eqs. (13) and (14). Thus, since β is given by eq. (A.4) when Q is equal to the identity, we have proved that eq. (13) applies to β-type coefficients as well. The same reasoning extends the proof to α-type coefficients.

Appendix B

General formulas for the coefficients of the p-RH

According to standard rules for products of density operators [32], eq. (12) yields

$$\begin{aligned}\alpha &= \langle\langle {}^pE^{123456\ldots(p+2)}_{341256\ldots(p+2)}\rangle\rangle + \langle\langle {}^pE^{12456\ldots(p+2)}_{14256\ldots(p+2)}\rangle\rangle \\ &\quad + \langle\langle {}^pE^{12356\ldots(p+2)}_{32156\ldots(p+2)}\rangle\rangle + \langle\langle {}^pE^{1256\ldots(p+2)}_{1256\ldots(p+2)}\rangle\rangle\,, \\ \beta &= \langle\langle {}^pE^{123456\ldots(p+2)}_{132456\ldots(p+2)}\rangle\rangle + \langle\langle {}^pE^{12456\ldots(p+2)}_{12456\ldots(p+2)}\rangle\rangle\,, \\ \mu &= \langle\langle {}^pE^{123456\ldots(p+2)}_{123456\ldots(p+2)}\rangle\rangle\,. \end{aligned} \tag{B.1}$$

Equation (13) enables us to transform the density operators of eqs. (B.1) into well ordered operators. Since an ordered density operator is given by a product of occupation numbers (see, e.g., [32]), we have that

$$\begin{aligned}\alpha &= -\tfrac{1}{8}\langle\langle n_1n_2n_3\ldots n_{p+2}\rangle\rangle - \langle\langle n_1n_2n_3\ldots n_{p+1}\rangle\rangle + \langle\langle n_1n_2n_3\ldots n_p\rangle\rangle\,, \\ \beta &= -\tfrac{1}{2}\langle\langle n_1n_2n_3\ldots n_{p+2}\rangle\rangle + \langle\langle n_1n_2n_3\ldots n_{p+1}\rangle\rangle\,, \\ \mu &= \langle\langle n_1n_2n_3\ldots n_{p+2}\rangle\rangle\,. \end{aligned} \tag{B.2}$$

Finally, the next expression [38] for the traces of occupation number operators in a $H^A(N,K)$ space,

$$\langle\langle n_1n_2n_3\ldots n_p\rangle\rangle = 2^p\sum_{i=0}^{p}\begin{bmatrix} p \\ i \end{bmatrix}\begin{bmatrix} 2(K-p) \\ N-p-i \end{bmatrix}, \tag{B.3}$$

gives us a set of three general, closed, formulas for the calculation of coefficients arising in the p-RH, for an arbitrary order p.

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