Reply to "Spin-adapted reduced Hamiltonian in view of the spectral-distribution method"

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In the preceding comment Nomura derived a general formula for traces of products of occupation number operators over finite-dimensional, N-electron, and spin-adapted spaces within the spectral-distribution method of nuclear physics. We supplement and generalize his result by giving recurrent relations which determine the traces in an alternative way. The relations are derived using simple techniques of atomic and molecular physics.

Nomura, in the preceding comment[1] (hereafter referred to as paper I) on our recent paper,[2] shows how approaches originating from different traditions may interact with each other and inspire new and more general formulations contributing in this way to a deeper understanding of the theoretical models. The analysis of Nomura, based on the spectral-distribution method of nuclear physics (for references see paper I), results in a closed-form expression for traces of certain products of the occupation number operators over finite-dimensional and spin-adapted many-electron spaces. Though it covers only a part of problems met in procedures aimed at the evaluation of matrix elements of reduced Hamiltonians, it is an important contribution to the theory. In this paper we supplement and generalize the results of Nomura,[1] presenting several recurrent formulas which determine an equivalent set of traces of products of the occupation number operators. We also give a new derivation of the final equation of Nomura. All the considerations are based on standard techniques of our approach.

It is convenient to define

$$W_q^r(S,N,K)=\langle n_1^2,n_2^2,\ldots,n_r^2,n_{r+1},n_{r+2},\ldots,n_{r+q}\rangle^{SNK}\,, \tag{1}$$

where symbols have the same meaning as in the previous papers.[1,2] Then the product calculated by Nomura[1] may be expressed as

$$G(p,q)=\left\langle \frac{n_1(n_1-1)}{2}\,\frac{n_2(n_2-1)}{2}\cdots\frac{n_r(n_r-1)}{2}\times n_{r+1}n_{r+2}\cdots n_{r+q}\right\rangle^{SNK}=2^{-r}\sum_{t=0}^{r}(-1)^t\begin{bmatrix} r\\ t\end{bmatrix}W_{q+t}^{r-t}(S,N,K)\,, \tag{2}$$

with $p=2r+q$.

Since

$$\left\langle \frac{n_1(n_1-1)}{2}F^1\right\rangle^{SNK}=\langle F^1\rangle^{S,N-2,K-1}\,, \tag{3}$$

$$\left\langle \frac{(n_1-1)(n_1-2)}{2}F^1\right\rangle^{SNK}=\langle F^1\rangle^{S,N,K-1}\,, \tag{4}$$

where F^1 is a function of the occupation numbers not containing n_1, then writing

$$n=1+\frac{n(n-1)}{2}-\frac{(n-1)(n-2)}{2}\,,$$

$$n^2=1+3\frac{n(n-1)}{2}-\frac{(n-1)(n-2)}{2}\,,$$

we get

$$W_q^r(S,N,K)=W_{q-1}^r(S,N,K)+W_{q-1}^r(S,N-2,K-1)-W_{q-1}^r(S,N,K-1) \tag{5}$$

and

$$W_q^r(S,N,K)=W_q^{r-1}(S,N,K)+3W_q^{r-1}(S,N-2,K-1)-W_q^{r-1}(S,N,K-1)\,, \tag{6}$$

with

$$W_0^0(S,N,K)=D(S,N,K)\,, \tag{7}$$

where $D(S,N,K)$ is the dimension of the space.[1,2] Combining Eqs. (5) and (6) we obtain two other relations:

$$W_q^{r+1}(S,N,K)-W_{q+1}^r(S,N,K)=2W_q^r(S,N-2,K-1) \tag{8}$$

and

$$W_{q-1}^{r+1}(S,N,K)-W_{q+1}^{r-1}(S,N,K)=2[W_{q-1}^r(S,N-2,K-1)+W_q^{r-1}(S,N-2,K-1)]\,, \tag{9}$$

which are particularly interesting because of their symmetry.

Since

$$\sum_{i=1}^{K}\langle n_i n_1^2 n_2^2\cdots n_r^2 n_{r+1}n_{r+2}\cdots n_{r+q}\rangle^{SNK}=NW_q^r(S,N,K)=r\langle n_1^3n_2^2\cdots n_r^2n_{r+1}n_{r+2}\cdots n_{r+q}\rangle^{SNK}+qW_{q-1}^{r+1}(S,N,K)+(K-r-q)W_{q+1}^r(S,N,K)\,, \tag{10}$$

we have

$$(3r-N)W_q^r-2rW_{q+1}^{r-1}+qW_{q-1}^{r+1}+(K-r-q)W_{q+1}^r=0\ , \tag{11}$$

where we used the identity[2]

$$\langle n_1^3F^1\rangle=3\langle n_1^2F^1\rangle-2\langle n_1F^1\rangle\ . \tag{12}$$

Equation (11) connects traces in the same space. By fixing either r or q it may be used as a recurrent relation determining certain sequences of the traces.

Now a set of recurrent equations expressing traces of products of the occupation number operators in terms of $D(i)\equiv D(S,N-2i,K-i)$ may be written as follows:

$$W_0^0(0)=D(0)\ , \tag{13}$$

$$W_{q+1}^0(0)=\frac{N-q}{K-q}W_q^0(0)-\frac{2q}{K-q}W_{q-1}^0(1)\ , \tag{14}$$

$$W_q^{r+1}(0)=W_{q+1}^r(0)+2W_q^r(1)\ , \tag{15}$$

where

$$W_q^p(i)\equiv W_q^p(S,N-2i,K-i)\ .$$

Equation (14) results directly from (11) and (1). Equations (13)–(15) determine traces of all products in a complete and unique way. In particular, as it results immediately from Eq. (3),

$$G(p,q)=W_q^0(r)\ . \tag{16}$$

Finally, $D(i)$ may be expressed as simple functions of S, N, and K using the Weyl-Paldus dimension formula.[3]

The closed-form expression for $W_q^0(0)$ may be obtained from Eq. (14) in a standard way. Iterating Eq. (14) we can observe that

$$W_q^0(0)=\sum_{j=0}^{[q/2]}(-1)^j a_j^q\frac{(N-2j)!(K-q)!}{(N-q)!(K-j)!}D(j)\ , \tag{17}$$

where a_j^q is a positive integer which depends on neither N nor K. Substituting Eq. (17) into Eq. (14), after some algebra, we get

$$a_j^{q+1}=a_j^q+2qa_{j-1}^{q-1}\ , \tag{18}$$

with condition

$$a_j^q=0\ \text{ if } j>\left[\frac{q}{2}\right]\ .$$

Equation (18) implies that

$$a_j^q=\frac{q!}{j!(q-2j)!}\ . \tag{19}$$

In order to get the expression for $W_q^0(r)$, i.e., the final equation of Nomura [(Eq. (24) of paper I], it is enough to replace, in Eq. (17), N by $N-2r$ and K by $K-r$.

Finally, we should comment on usefulness of the recurrent relations as compared to the closed-form expression as it is given by Nomura.[1] The closed-form expression is certainly the most compact way of determining the traces. It is also most useful if the value of a specific trace corresponding to $r=0$ is to be found. On the other hand, when a set of values of the traces is needed, then using recurrent relations is usually simpler. In particular it is often the case when structuring computer programs. Also, obtaining traces for $r\neq 0$ is much easier using our recurrent relation (15) than the inverted Eq. (2), i.e.,

$$W_q^r(0)=\sum_{t=0}^{r}2^t\begin{bmatrix} r\\ t\end{bmatrix}W_{q+r-t}^0(t)\ . \tag{20}$$

Recurrent relations may also be considered as a set of identities. In our case these identities may be helpful in studying general properties of quantities being expressible in terms of the traces as, e.g., the spin-adapted reduced Hamiltonian matrix elements or moments of spectral density distribution.

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