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Group projector generalization of the Dirac–Heisenberg model

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Abstract. The general form of the operators commuting with the ground representation (appearing in many physical problems within the single-particle approximation) of the group is found. With the help of the modified group projector technique, this result is applied to a system of identical particles with spin-independent interaction, to derive the Dirac–Heisenberg Hamiltonian and its effective space for arbitrary orbital occupation numbers and arbitrary spin. This gives transparent insight into the physical contents of this Hamiltonian, showing that formal generalizations with spin greater than $\frac{1}{2}$ involve non-trivial additional physical assumptions.

1. Introduction

Considering systems of identical electrons interacting by Coulomb forces only, Dirac found [1] that the effective Hamiltonian can be expressed in the spin space only: $H = U + \sum_{k<l} J_{kl} \boldsymbol{s}_k \cdot \boldsymbol{s}_l$, where $\boldsymbol{s}_i$ is a vector of the Pauli matrices related to the spin in the ith site. The aim of this paper is to present a rigorous derivation of the Dirac–Heisenberg Hamiltonian for any spin, within the framework of the original physical assumptions. This means that an arbitrary spin-independent interaction of the identical particles is considered. Then, due to the perturbative approach, the Hamiltonian is approximately reduced in the subspaces of the orbital state space spanned by the vectors with the same occupation number. Such a subspace carries a special induced type representation (ground representation) of the permutational group, commuting with the reduced Hamiltonian. The general form of the operator commuting with the ground representation is derived in section 2 and the result is applied to the considered Hamiltonian in section 3, yielding its form in the orbital many-particle factor space. Finally, the required form of the Hamiltonian is obtained in section 4, by a restriction to the relevant (symmetrized or antisymmetrized) subspace of the total space. This step is based on the modified group projector technique for the induced representations.

The result generalizes the original derivation with respect to spin and occupation numbers. Nevertheless, the physical framework remains the same, in contrast to the formal generalizations appearing in various theories of magnetic materials [2], when in the Dirac–Heisenberg Hamiltonian only the values of spin and the interaction coefficients are appropriately modelled.

The rest of the introduction gives a necessary reminder on the modified group projector technique. Let $D(\boldsymbol{G})$ be the representation of the group $\boldsymbol{G}$ in the space $\mathcal{H}_D$, decomposing into the irreducible components $D^{(\mu)}(\boldsymbol{G})$ as $D(\boldsymbol{G}) = \oplus_{\mu=1}^{r} a_\mu D^{(\mu)}(\boldsymbol{G})$ (a_μ is the frequency number of $D^{(\mu)}(\boldsymbol{G})$). The symmetry-adapted [3, 4] (or standard) basis $\{|\mu t_\mu m\rangle | \mu = 1, \ldots, r; t_\mu = 1, \ldots, a_\mu; m = 1, \ldots, |\mu|\}$ ($|\mu|$ denotes the dimension of $D^{(\mu)}(\boldsymbol{G})$) in $\mathcal{H}_D$ is defined by the following condition:

$$D(g)|\mu t_\mu m\rangle = \sum_{m'=1}^{|\mu|} D^{(\mu)}_{m'm}(g)|\mu t_\mu m'\rangle. \tag{1}$$

To find this basis [5], the auxiliary representation $\Gamma^\mu(\boldsymbol{G}) \stackrel{\text{def}}{=} D(\boldsymbol{G}) \otimes D^{(\mu)*}(\boldsymbol{G})$ in the space $\mathcal{H}_D \otimes \mathcal{H}^{(\mu)^*}$ is constructed for each irreducible component $D^{(\mu)}(\boldsymbol{G})$ (with $a_\mu > 0$) of $D(\boldsymbol{G})$. Here, $D^{(\mu)*}(\boldsymbol{G})$ is the dual representation of $D^{(\mu)}(\boldsymbol{G})$; in fact, it is the conjugated one, since the finite permutational groups and their unitary representations are considered. The range of the modified projector $G(\Gamma^\mu) \stackrel{\text{def}}{=} (1/|\boldsymbol{G}|)\sum_g \Gamma^\mu(\boldsymbol{G})$ is the (a_μ-dimensional) subspace $\mathcal{F}^\mu$ of the fixed points for the representation $\Gamma^\mu(\boldsymbol{G})$. For the arbitrary basis $\{|\mu t_\mu\rangle | \mu = 1, \ldots, a_\mu\}$ of $\mathcal{F}^\mu$, the subbasis $\{|\mu t_\mu m\rangle | m = 1, \ldots, |\mu|\}$ is found by the partial scalar product with the standard vectors $|\mu m\rangle$ of the irreducible representation

$$|\mu t_\mu m\rangle = \langle \mu m | \mu t_\mu\rangle. \tag{2}$$

If $\boldsymbol{G}$ is the symmetry group of the Hamiltonian H (thus $[D(g), H] = 0$ for each $g \in \boldsymbol{G}$), then taking for $|\mu t_\mu\rangle$ an eigenbasis of $H \otimes I_\mu$ (I_μ is the identity in $\mathcal{H}^{(\mu)^*}$), equation (2) gives the symmetry-adapted eigenbasis for H: $H|\mu t_\mu m\rangle = E_{\mu t_\mu}|\mu t_\mu m\rangle$.

The representations involved in this paper are of the induced type. Precisely, let $\boldsymbol{K}$ be a subgroup of $\boldsymbol{G}$ with the transversal $\boldsymbol{Z} = \{z_t | t = 0, \ldots, |\boldsymbol{Z}| - 1\}$ (z_0 is the identity of the group, $|\boldsymbol{Z}| = |\boldsymbol{G}|/|\boldsymbol{K}|$). Then $D(\boldsymbol{G}) = \Delta(\boldsymbol{G}) \otimes d(\boldsymbol{G})$, where $\Delta(\boldsymbol{G}) = \Delta'(\boldsymbol{K} \uparrow \boldsymbol{G})$ is an induced representation and $d(\boldsymbol{G})$ is some other representation of $\boldsymbol{G}$. In this case the modified projectors can be reduced [6] to the subgroup modified projector $K(\gamma^\mu)$ for the representation $\gamma^\mu(\boldsymbol{K}) = \Delta'(\boldsymbol{K}) \otimes d(\boldsymbol{G} \downarrow \boldsymbol{K}) \otimes D^{(\mu)*}(\boldsymbol{G} \downarrow \boldsymbol{K})$ in $\mathcal{H}_{\gamma^\mu} = \mathcal{H}_{\Delta'} \otimes \mathcal{H}_d \otimes \mathcal{H}^{(\mu)^*}$:

$$G(\Gamma^\mu) = B^\mu\{E^{00} \otimes K(\gamma^\mu)\}B^{\mu^\dagger}. \tag{3}$$

Here, $B^\mu \stackrel{\text{def}}{=} (1/\sqrt{|\boldsymbol{Z}|})\sum_{z_t} E^{t0} \otimes I_{\Delta'} \otimes d(z_t) \otimes D^{(\mu)^*}(z_t)$ is partial isometry and $E^{t0} = |z_t\rangle\langle z_0|$ are $|\boldsymbol{Z}|$-dimensional square matrices with only one non-vanishing element $(E^{t0})_{t0} = 1$. It appears that the range of $K(\gamma^\mu)$ (the subspace in $\mathcal{H}_{\gamma^\mu}$) is the effective space, while the effective Hamiltonian is $H^\mu = B^{\mu^\dagger}(H \otimes I_\mu)B^\mu K(\gamma^\mu)$. Indeed, the symmetry-adapted eigensubbasis $|\mu t_\mu m\rangle$ corresponding to the irreducible representation $D^{(\mu)}(\boldsymbol{G})$ is found by (2) with the vectors $|\mu t_\mu\rangle = B^{\mu^\dagger}|\mu t_\mu\rangle^0$, where $|\mu t_\mu\rangle^0$ are the eigenvectors of H^μ from the range of $K(\gamma^\mu)$: $H^\mu|\mu t_\mu\rangle^0 = E_{\mu t_\mu}|\mu t_\mu\rangle^0$.

2. Invariants of ground representations

If $\boldsymbol{K}$ is the subgroup in the finite group $\boldsymbol{G}$, its left transversal $\boldsymbol{Z}$ gives the coset partition $\boldsymbol{G} = \sum_t z_t\boldsymbol{K}$. Therefore, to each element $g \in \boldsymbol{G}$ there corresponds one element $\overline{g}$ of $\boldsymbol{Z}$: there are uniquely defined $k \in \boldsymbol{K}$ and $z_t \in \boldsymbol{Z}$, such that $g = z_t k$, and z_t is denoted by $\overline{g}$. Together with this coset decomposition, the subgroup $\boldsymbol{K}$ gives the double-coset decomposition [7–9] of $\boldsymbol{G}$ over $\boldsymbol{K}$: $\boldsymbol{G} = \sum_\lambda \boldsymbol{K}z_\lambda\boldsymbol{K}$. Each double coset decomposes onto one or more cosets, $\boldsymbol{K}z_\lambda\boldsymbol{K} = \sum_m z_{\lambda m}\boldsymbol{K}$. Thus, the double coset representatives can be chosen among the elements of the transversal $\boldsymbol{Z}$. The double-coset decomposition enables one to define for each $g \in \boldsymbol{G}$ its double-coset representative z_λ by $g = kz_\lambda k'$ ($k, k' \in \boldsymbol{K}$), denoted also as $\overline{\overline{g}}$.

Furthermore, each $g \in \boldsymbol{G}$, and $z_m \in \boldsymbol{Z}$ define uniquely $z_s \in \boldsymbol{Z}$ and $k \in \boldsymbol{K}$, such that $gz_m = z_s k$. Obviously, with the above notational convention, $z_s = \overline{gz_m}$, and the left (permutational) action of $\boldsymbol{G}$ over $\boldsymbol{Z}$ becomes $g : z_m \mapsto \overline{gz_m}$. This action is faithfully represented by the linear operators of the left ground representation $L(\boldsymbol{G}) = \mathbf{1}(\boldsymbol{K} \uparrow \boldsymbol{G})$ in the $|\boldsymbol{Z}|$-dimensional vector space, $\mathcal{Z}$: each element of $z_m \in \boldsymbol{Z}$ is mapped to the basis vector $|z_m\rangle$. The operators of $\boldsymbol{G}$ are defined by $L(g)|z_m\rangle \stackrel{\text{def}}{=} |\overline{gz_m}\rangle$, i.e. $L(g) = \sum_m |\overline{gz_m}\rangle\langle z_m|$. The homomorphism condition $L(gg') = L(g)L(g')$ is easily checked.

Also, the right multiplication $z_m g = z_s k$ introduces the 'right' operators $R(g)$: $\langle z_m|R(g) \stackrel{\text{def}}{=} \langle\overline{z_m g}|$, or $R(g) = \sum_m |z_m\rangle\langle\overline{z_m g}|$. These operators form an antirepresentation $(R(g)R(g') = R(g'g))$ if and only if $\boldsymbol{K}$ is an invariant subgroup. Since $\overline{z_s z_m k} = \overline{z_s z_m}$, it turns out that $R(z_m k) = R(z_m)$ for each $k \in \boldsymbol{K}$, i.e. that the mapping $g \mapsto R(g)$ is a function over the cosets of $\boldsymbol{K}$.

All the operators $L(g)$ and $R(g)$ are in the basis $\{|z_m\rangle\}$ given by the real matrices, with elements 0 or 1. In particular, for the unitary (in fact orthogonal) matrices $L(g)$ this yields $L(g)^T = L(g^{-1})$.

Now, the condition that the operator A acting in $\mathcal{Z}$ is invariant of $\boldsymbol{G}$ means that $[A, L(g)] = 0$ for each g in $\boldsymbol{G}$. Such an operator has a very special form.

Theorem 1. *Any invariant operator A in $\mathcal{Z}$ is of the form $A = \sum_{g\in\boldsymbol{G}} \alpha(\overline{\overline{g}})R(g)$, where $\alpha(\overline{\overline{g}})$ is a function over double cosets of $\boldsymbol{K}$ in $\boldsymbol{G}$ (i.e. these constants can be chosen independently, one for each double coset).*

The proof consists of two parts. At first, the commutation with the operators $L(z_m)$ representing the transversal is used: because of $L(z_m)|z_0\rangle = |\overline{z_m z_0}\rangle = |z_m\rangle$, one has $A = \sum_{m,n}\langle m|A|n\rangle|m\rangle\langle n| = \sum_{mn}\langle z_0|L^T(z_m)A|n\rangle|m\rangle\langle n|$. Since z_m^{-1} is also an element of $\boldsymbol{G}$, it commutes with A, and

$$A = \sum_{mns}\langle z_0|A|z_s\rangle\langle z_s|L^T(z_m)|z_n\rangle|z_m\rangle\langle z_n| = \sum_{ms} A^{0s}|z_m\rangle\langle\overline{z_m z_s}|$$

giving finally $A = \sum_s A^{1s}R(z_s)$. Consequently, the matrix of the invariant A is completely determined by its first row. Secondly, the subgroup elements are employed; for each double-coset representative z_λ and each element $k \in \boldsymbol{K}$ it holds

$$A^{0\lambda} = \langle z_0|A|z_\lambda\rangle = \langle z_0|L(k)A|z_\lambda\rangle = \langle z_0|AL(k)|z_\lambda\rangle = \langle z_0|A|\overline{kz_\lambda}\rangle.$$

When k goes over $\boldsymbol{K}$, all the elements $\overline{kz_\lambda}$ go over the coset representatives of the whole double coset of z_λ, meaning that the matrix elements A^{0s} and A^{0t} must be the same if z_t and z_s are from the same double coset. Together with the previous conclusion this gives $A = \sum_\lambda A^{0\lambda}\sum_m R(z_{\lambda m})$. To complete the proof, it remains to recall that the right operators are the same for the elements of the same coset.

From theorem 1 it immediately follows that the number of linearly independent invariants is equal to the number of double cosets of $\boldsymbol{K}$. Precisely, to each double coset represented by z_λ, there corresponds the invariant $A_\lambda = \sum_{g\in\boldsymbol{K}z_\lambda\boldsymbol{K}} R(g)$. In the special case, when $\boldsymbol{K} = \{e\}$, the trivial subgroup containing the identity only, the ground representation is the regular representation of the group; since in this case each element of the group is itself one coset and one double coset, there are exactly $|\boldsymbol{G}|$ independent invariants, each of them being one of the operators $R(g)$ (in this case $R(g^{-1})$ form the right regular representation of $\boldsymbol{G}$, being equivalent to the left one $L(\boldsymbol{G})$), and all the left operators commute with all the right ones.

3. Generalized Dirac–Heisenberg Hamiltonian

Let $\mathcal{H} = \mathcal{H}_o \otimes \mathcal{H}_s$ be the quantum mechanical state space of some particle, where $\mathcal{H}_o$ and $\mathcal{H}_s$ are the orbital and the spin factor spaces. Then, for the system of N particles the tensor powers $\mathcal{H}_o^N \stackrel{\text{def}}{=} \mathcal{H}_o \otimes \cdots \otimes \mathcal{H}_o$ (N times) and $\mathcal{H}_s^N$ are constructed, and in the space $\mathcal{H}^N = \mathcal{H}_o^N \otimes \mathcal{H}_s^N$ the symmetric (bosons) or antisymmetric (fermions) part are considered as the state space of the total system. If $\{|i\rangle | i = 1, \ldots, |o|\}$ is a basis in $\mathcal{H}_o$, then $\{|i_1, \ldots, i_n\rangle \stackrel{\text{def}}{=} |i_1\rangle \cdots |i_N\rangle | i_1, \ldots, i_N = 1, \ldots, |o|\}$ is a basis in $\mathcal{H}_o^N$. Each of this vectors defines the occupation number vector $\boldsymbol{n} = (n_1, \ldots, n_{|o|})$, with the component n_i showing the number of particles in the state $|i\rangle$.

Each permutation π of the symmetric group S_N, is represented by the operator $\Delta(\pi)$, defined by the action $\Delta(\pi)|i_1, \ldots, i_N\rangle \stackrel{\text{def}}{=} |i_{\pi^{-1}1}, \ldots, i_{\pi^{-1}N}\rangle$. This action does not change the occupation number of the basis vectors, and the orbit of the action gives the set of the basis vectors with the same occupation numbers. Thus, each orbit is uniquely defined by the occupation number and spans the subspace $\mathcal{H}_{\boldsymbol{n}}^N$ invariant for the representation $\Delta(S_N)$. Consequently, in $\mathcal{H}_{\boldsymbol{n}}^N$ $\Delta(S_N)$ is reduced to the representation $\Delta_{\boldsymbol{n}}(S_N)$. Its dimension is equal to the order of the orbit with the occupation number $\boldsymbol{n}$, $|\Delta_{\boldsymbol{n}}| = N!/(n_1! \cdots n_{|o|}!)$, since the stabilizer of the vector with the occupation number $\boldsymbol{n}$ is $S_N^{\boldsymbol{n}} = S_{n_1} \otimes \cdots \otimes S_{n_{|o|}}$. Note that, being induced from the trivial representation of the stabilizer, $\Delta_{\boldsymbol{n}}(S_N) = \mathbf{1}(S_N^{\boldsymbol{n}} \uparrow S_N)$, $\Delta_{\boldsymbol{n}}(S_N)$ is a ground representation [7].

To summarize, the space $\mathcal{H}_o^N$ is decomposed into the orthogonal sum $\mathcal{H}_o^N = \oplus_{\boldsymbol{n}} \mathcal{H}_{\boldsymbol{n}}^N$. In each of these subspaces acts the ground representation $\Delta_{\boldsymbol{n}}(S_N)$, and the partial reduction of the representation $\Delta(S_N)$ is obtained: $\Delta(S_N) = \oplus_{\boldsymbol{n}} \Delta_{\boldsymbol{n}}(S_N)$.

Let H be a spin-independent Hamiltonian of the system of N identical particles. It is written in the form $H = H_1 + H_2$, where $H_1 = \sum_{s=1}^N h_s$ is the non-interacting part. Here, h_i is a one-particle Hamiltonian, i.e. the operator in the space $\mathcal{H}_o$, while $H_2 = \sum_{s<t} V_{st}$ describes two-particle interaction. Since H commutes with the operators $\Delta(S_N)$, all h_s must be equivalent: the full form of h_s is the tensor product of the identity operators in all the spaces except in the sth one, where the corresponding factor is the same, for example, h. Analogously, all the operators V_{st} are the same except that their non-trivial action is reduced to the different pair of spaces.

If the basis $\{|i\rangle\}$ is chosen as the eigenbasis of h (with the eigenvalues ϵ_i), then the vectors of the subspace $\mathcal{H}_{\boldsymbol{n}}^N$ are the eigenvectors of H_1 for the eigenvalue $E_{\boldsymbol{n}} = \sum_{i=1}^d n_i \epsilon_i$. Although this subspace need not be invariant for H_2, the approximation $H_2 \approx \oplus_{\boldsymbol{n}} H_{2\boldsymbol{n}}$, with $H_{2\boldsymbol{n}} = P_{\boldsymbol{n}} H_2 P_{\boldsymbol{n}}$ ($P_{\boldsymbol{n}}$ stands for the projector onto $\mathcal{H}_{\boldsymbol{n}}^N$) enables the perturbative approach, involving the eigenproblems of the operators $H_{2\boldsymbol{n}}$. Since H_2 is invariant of S_N in the whole space $\mathcal{H}_o^N$, the operators $H_{2\boldsymbol{n}}$ are also S_N-invariants, i.e. they commute with the corresponding representation $\Delta_{\boldsymbol{n}}(S_N)$. Recalling that this is the ground representation, theorem 1 gives the most general form

$$H_{2\boldsymbol{n}} = \sum_{\pi \in S_N} \alpha(\overline{\overline{\pi}}) R_{\boldsymbol{n}}(\pi). \tag{4}$$

Here, $R_{\boldsymbol{n}}(\pi)$ are the right operators of $\Delta_{\boldsymbol{n}}(\pi)$, while the coefficients α are equal for all the permutations from the same double coset of $S_N^{\boldsymbol{n}}$.

Until now, only the orbital space $\mathcal{H}_o^N$ has been considered, since the Hamiltonian acts trivially in the spin factors. Nevertheless, the particles are identical, and either the symmetrized or the antisymmetrized part of the total space $\mathcal{H}^N$ is to be considered. The orbital occupation number decomposition yields the decomposition of the total space: $\mathcal{H}^N = \oplus_{\boldsymbol{n}} \mathcal{H}_{\boldsymbol{n}}^N \otimes \mathcal{H}_s^N$. Using an arbitrary basis $\{|\sigma\rangle | \sigma = 1, \ldots, 2s+1\}$ in the single-particle spin space $\mathcal{H}_s$, the representation $d(S_N)$ in $\mathcal{H}_s^N$ is defined analogously to $\Delta(S_N)$ in $\mathcal{H}_o^N$: $d(\pi)|\sigma_1, \ldots, \sigma_N\rangle \stackrel{\text{def}}{=} |\sigma_{\pi^{-1}1}, \ldots, \sigma_{\pi^{-1}N}\rangle$, and in the total space the permutation π is represented by the operator $\Delta(\pi) \otimes d(\pi)$. Obviously the subspaces $\mathcal{H}_{\boldsymbol{n}}^N \otimes \mathcal{H}_s^N$ are invariant for the action of $\Delta \otimes d$, and the modified group projector of the irreducible representation $D^{(\mu)}(S_N)$,

$$S_N(\Delta\otimes d\otimes D^{(\mu)*}) = \frac{1}{N!}\sum_{\pi}\Delta(\pi)\otimes d(\pi)\otimes D^{(\mu)*}(\pi) = \oplus_{\boldsymbol{n}} S_N(\Delta_{\boldsymbol{n}}\otimes d\otimes D^{(\mu)*}) \tag{5}$$

treats each of these subspaces independently. Therefore, in each subspace $\mathcal{H}_{\boldsymbol{n}}^N\otimes\mathcal{H}_s^N$ there is the subspace $\mathcal{H}_{\boldsymbol{n}s}^{\mu}$ corresponding to the representation $D^{(\mu)}(S_N)$. It is spanned by the standard subbasis $\{|\mu t_\mu m\rangle\}$, obtained by (2) from any basis $\{|\boldsymbol{n};\mu t_\mu\rangle\}$ of the range $\mathcal{F}_{\boldsymbol{n}}^{\mu}$ of the projector $S_N(\Delta_{\boldsymbol{n}}\otimes d\otimes D^{(\mu)*})$; obviously, $\mathcal{F}_{\boldsymbol{n}}^{\mu}$ is the intersection of $\mathcal{H}_{\boldsymbol{n}}^N\otimes\mathcal{H}_s^N\otimes\mathcal{H}^{(\mu)^*}$ and the range $\mathcal{F}^{\mu}$ of the projector (5). In particular, taking the identity and the alternating representations, $D^{(\pm)}(\pi) = (\pm)^{\pi}$ (as usual, π in the exponent denotes the parity of π) for $D^{(\mu)}(S_N)$, the projector (5) becomes the symmetrizer and antisymmetrizer, respectively; in these cases of one-dimensional irreducible representations $\mathcal{F}_{\boldsymbol{n}}^{\pm}$ is itself the subspace $\mathcal{H}_{\boldsymbol{n}s}^{\pm}$.

4. Restriction to the relevant subspace

Since the involved representations are of the induced type, the modified group projector technique isomorphically relates by equation (3) the subspace $\mathcal{F}_{\boldsymbol{n}}^{\mu}$ of $\mathcal{H}_{\boldsymbol{n}}^N\otimes\mathcal{H}_s^N\otimes\mathcal{H}^{(\mu)^*}$ to the effective subspace, being the range of the subgroup projector $\boldsymbol{K}(\gamma^{\mu})$ in $\mathcal{H}_s^N\otimes\mathcal{H}^{(\mu)^*}$ (since $\Delta'(\boldsymbol{K})$ is a trivial representation). Of course, the effective Hamiltonian $H_{2\boldsymbol{n}}^{\mu}$ acts in the space $\mathcal{H}_s^N\otimes\mathcal{H}^{(\mu)^*}$ with the range contained in $\mathcal{F}_{\boldsymbol{n}}^{\mu}$. In particular, for the physically important representations $D^{(\pm)}(S_N)$, the effective Hamiltonian $H_{2\boldsymbol{n}}^{\pm}$ acts in the spin space $\mathcal{H}_s^N$, as well as $\boldsymbol{K}(\gamma^{\pm})$.

Precisely, in the considered context $\boldsymbol{G} = S_N$, $\boldsymbol{K} = S_N^{\boldsymbol{n}}$, $\Delta'(\boldsymbol{K}) = \mathbf{1}(S_N^{\boldsymbol{n}})$ and $d(S_N)$ is the permutational representation in the spin space. Thus,

$$B_{\boldsymbol{n}}^{\mu} = \frac{1}{\sqrt{|\boldsymbol{Z}|}}\sum_t |z_t\rangle\langle z_0|\otimes d(z_t)\otimes D^{(\mu)*}(z_t)$$

(with the omitted number 1 standing for Δ'). Then, skipping the factor $E^{00} = |z_0\rangle\langle z_0|$ (this only gives the space of the action of $H_{2\boldsymbol{n}}^{\mu}$), one finds

$$B_{\boldsymbol{n}}^{\mu^\dagger}(H_{2\boldsymbol{n}}\otimes I_\mu)B_{\boldsymbol{n}}^{\mu} = \frac{1}{N!}\sum_{\pi}\sum_{p,t}\alpha(\overline{\overline{\pi}})\langle z_t|R(\pi)|z_p\rangle d(z_t^{-1}z_p)\otimes D^{(\mu)*}(z_t^{-1}z_p).$$

The matrix element of $R(\pi)$ is obviously $\langle\overline{z_t\pi}|z_p\rangle = \delta_{z_p,\overline{z_t\pi}}$ (Kronecker delta). When the sum over $\pi = z_q\kappa$ is decomposed onto the sums over the transversal (q) and stabilizer (κ), the equality $\overline{z_tz_q\kappa} = \overline{z_tz_q}$ for $\kappa\in S_N^{\boldsymbol{n}}$ shows that all the terms are independent of κ. Thus

$$B_{\boldsymbol{n}}^{\mu^\dagger}(H_{2\boldsymbol{n}}\otimes I_\mu)B_{\boldsymbol{n}}^{\mu} = \frac{1}{|\boldsymbol{Z}|}\sum_{q,t}\alpha(\overline{\overline{z_q}})d(z_t^{-1}\overline{z_tz_q})\otimes D^{(\mu)*}(z_t^{-1}\overline{z_tz_q}).$$

Since the element $z_t^{-1}\overline{z_tz_q}$ can be written in the form $z_q\kappa'$ (i.e. it is from the coset represented by z_q), multiplication by $S_N^{\boldsymbol{n}}(d\otimes D^{(\mu)^*})$ gives

$$H_{2\boldsymbol{n}}^{\mu} = \frac{|\boldsymbol{Z}|}{N!}\sum_q\sum_\kappa\alpha(\overline{\overline{z_q}})d(z_q\kappa)\otimes D^{(\mu)*}(z_q\kappa)$$

and finally,

$$H_{2\boldsymbol{n}}^{\mu} = \frac{1}{n_1!\cdots n_{|o|}!}\sum_{\pi}\alpha(\overline{\overline{\pi}})d(\pi)\otimes D^{(\mu)*}(\pi). \tag{6}$$

This relation is, in fact, the most general form of the μth component of the permutational invariant Hamiltonian acting in $\mathcal{H}_n^N \otimes \mathcal{H}_s^N$, being trivial in $\mathcal{H}_s^N$. Note that this operator acts in the space isomorphic to the direct product of $\mathcal{H}_s^N$ and the space of the representation $D^{(\mu)}(S_N)$. Still, the range of the projector $K(\gamma^\mu) = [1/(n_1! \cdots n_{|o|}!)] \sum_\kappa \gamma^\mu(\kappa)$ is the effective part of this space (its orthocomplement is from the kernel of H_{2n}^μ). Finally, let me stress again that the coefficients α can be deliberately chosen only one for each double coset of S_N^n.

Two simplifications are physically relevant. First, as has been mentioned already, the irreducible representation $D^{(\mu)}(S_N)$ is actually either the symmetric or the antisymmetric one, giving

$$H_{2n}^{\pm} = \frac{1}{n_1! \cdots n_{|o|}!} \sum_\pi (\pm)^\pi \alpha(\overline{\overline{\pi}}) d(\pi). \tag{7}$$

In these cases, the effective space of $H_{2n}^{\pm}$ is the subspace in the spin space $\mathcal{H}_s^N$.

The second one is that only two-particle interactions are considered, meaning that only the permutations of at most two particles are involved in (4). With τ_{kl} denoting the transposition of particles k and l, expressions (4) and (7) become $H_{2n} = \alpha(e)I + \sum_{l<k} \alpha(\overline{\overline{\tau_{lk}}}) R_n(\tau_{lk})$, and

$$H_{2n}^{\pm} = \frac{1}{n_1! \cdots n_{|o|}!} \left[\alpha(e)I \pm \sum_{k<l} \alpha(\overline{\overline{\tau_{kl}}}) d(\tau_{kl}) \right]. \tag{8}$$

5. Concluding remarks

Originally, the Hamiltonian (8) is derived [1] for the case when the orbital occupation numbers n_i are at most 1, meaning that S_N^n is the trivial subgroup $\{e\}$, and therefore $\Delta_n(S_N)$ is the regular ($N!$-dimensional) representation of S_N. In this case the coefficients α can be chosen arbitrarily, since each element of S_N is itself one double coset. Further, in this case the group projector $K(\gamma^{\pm})$ is the identity operator in the space $\mathcal{H}_s^N$, meaning that the whole spin space is efficient.

Of course, for spin $s = \frac{1}{2}$ the transposition τ_{ij} is in the space H_s^N represented by the operator $d(\tau_{ij}) = \frac{1}{2}(I + \boldsymbol{s}_i \cdot \boldsymbol{s}_j)$, and (8) takes the usual form

$$H_{2n}^{-} = U + \sum_{k<l} J(\overline{\overline{\tau_{kl}}}) \boldsymbol{s}_k \cdot \boldsymbol{s}_l. \tag{9}$$

Although the same form is frequently used [2] with the spin operators for $s \neq \frac{1}{2}$, these formal generalizations do not preserve the original physical meaning of the Heisenberg–Dirac Hamiltonian: the resulting operator cannot be derived from the pure orbital interaction of the identical particles (for higher spin the transpositions cannot be expressed by the spin matrices in the same form). Even for $s = \frac{1}{2}$, the interaction coefficients can only be chosen independently for any pair of sites for the occupation numbers $n_i \leqslant 1$; in other cases, they must be the same over the same double coset of S_N^n, while the relevant space is only a subspace of the total spin space $\mathcal{H}_s^N$, which can be found easily with help of the subgroup projector $S_N^n(d \otimes D^{(-)})$. Indeed, using the direct product factorization of the group S_N^n, the projector can be written in the form $S_N^n(d \otimes D^{(-)}) = \otimes_{i=1}^{|o|} S_{n_i}(d \otimes D^{(-)})$. Each of the factors may be found straightforwardly; moreover, only the generating transpositions may be involved [5]. This simple restriction to the relevant space may be used to reduce the time taken in various numerical calculations.

Finally, let me emphasize that the general form of the Hamiltonian acting in the space of the ground representation of the symmetry group (thus commuting with it), given by theorem 1 is the important result, independent of the Dirac–Heisenberg Hamiltonian. Indeed, this situation occurs in the context of the single-particle approximations [9], e.g. when the tight-binding electronic levels, spin waves or normal vibrations modes are calculated: then the symmetry group action can be factorized into a permutational part $D^{\mathrm{P}}(\boldsymbol{G})$ and an interior part $D^{\mathrm{int}}(\boldsymbol{G})$. The latter is related to the phenomena considered (this is a polar and axial vector representation of the group in the case of normal modes and spin waves, and the representation carried by the atomic orbitals from the same site in the electronic tight-binding calculations). The former describes the geometry of the system, showing how the transformations of the group map one site into another, and this is always the ground representation induced from the site stabilizer. Again theorem 1 can be used to find the general form of the Hamiltonian, restricting possible theoretical models and enabling further exact simplifications along to these presented in the context of the Dirac–Heisenberg problem.

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