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COMMENT

A comment on the modified group projector technique

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Abstract. It is shown that within the modified group projector technique the symmetry adapted bases can be determined using only the representatives of the generators for any group (not only for the factorizable ones, as has been proposed recently).

It has been shown recently [1] that the symmetry adapted basis for the representation $D'(G)$ of the group G can be found with use of the group projectors $G(D) := \frac{1}{G}\sum_{g\in G} D(g)$, for the representations $D(G) = D^{(\mu)*}(G) \otimes D'(G)$ ($D^{(\mu)}(G)$ being the irreducible components of $D'(G)$; unitarity of the representations has been assumed). For each subset Y, the operators $Y(D) := \frac{1}{Y}\sum_{g\in Y} D(g)$ have been introduced. It has been shown that if the group G is the product of its subgroups H and K, $G = HK$ (for each $g \in G$ there are elements $h \in H$ and $k \in K$ such that $g = hk$), then the subgroup projectors $H(D)$ and $K(D)$ commute, and their product is the group projector $G(D)$. For the groups factorizable to the cyclic subgroups, $G = G_1G_2\ldots$, G_i being generated by g_i, $G_i(D)$ is the eigenprojector for the eigenvalue 1 of the operator $D(g_i)$. Thus the whole problem has been reduced to the calculation of these eigenprojectors.

Although the groups with such factorizability frequently appear in physics, there are counterexamples (e.g. quaternionic group K_8, or some of the non-symorphic space groups). So, it is desirable to generalize the method to encompass all the cases. Let $\mathcal{F}(A)$ and $F(A)$ denote the subspace of the fixed points of the operator A ($\mathcal{F}(A) := \{x \in \mathcal{H}|Ax = x\}$), and the projector on this subspace. Given the projectors P_i ($i = 1, \ldots, n$), with the ranges $\mathcal{F}(P_i)$, the subspace of their common fixed points is the intersection $\mathcal{F} = \cap_i \mathcal{F}(P_i)$. The projector F on this subspace is equal to the product $\prod_i P_i$ if and only if P_i mutually commute. Most generally, it can be shown that $F = F(\prod_i P_i)$ (the order of the projectors in the product is irrelevant): if $x \in \mathcal{F}$ then $P_i x = x$ for each i, and $(\prod_i P_i)x = x$, i.e. $x \in \mathcal{F}(\prod_i P_i)$; also, since the projectors decrease the norm of the vectors, $\|P_i y\| = \|y\|$ if and only if $y \in \mathcal{F}(P_i)$, $x \in \mathcal{F}(\prod_i P_i)$ means that x is in $\mathcal{F}(P_i)$ for each i, and therefore in $\mathcal{F}$.

Applying this remark to the groups, to each subset Y there is a corresponding projector $Y_F(D) := F(Y(D))$. This strengthens theorem 3 in [1], revealing a kind of morphism between the subsets and the corresponding projectors:

Theorem 1. Let $D(G)$ be a unitary representation of the group G.

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(i) If $Y^{-1} := \{y^{-1} | y \in Y\}$, then $(Y^{-1})_F(D) = (Y(D)^\dagger)_F = Y_F(D)$.

(ii) For closed subset Y (i.e. $YY = Y$) in G, $Y_F = Y(D)$.

(iii) For any two subsets X and Y in G, $(X \vee Y)_F(D) = F(X_F(D)Y_F(D))$ (here $X \vee Y$ is the subgroup generated by X and Y).

(iv) If $\{g_1, \ldots, g_n\}$ is the set of the generators of G, then $G(D) = F(\prod_{i=1}^n F(D(g_i)))$.

The last statement is technically the most important: the determination of the symmetry adapted bases for each group with n generators reduces to the calculation of $n+1$ projectors. This is simply the problem of solving the D-dimensional systems of linear equations of the type $Ax = x$, and no summation over group is involved.

Some additional relations can be useful in these calculations. Knowing the projectors $F(D(g_i))$, the group projector can be found as $G(D) = \lim_{N\to\infty}(\prod_{i=1}^n F(D(g_i)))^N$. Further, since $D(g_i)$ is a unitary operator, there exists a unique Hermitean operator H_i with the eigenvalues from the interval $[0, 2\pi)$, such that $D(g_i) = e^{iH_i}$. It is obvious that its null-space $\mathcal{N}(H_i) = \{x \in \mathcal{H} | H_i x = 0\}$ is equal to $\mathcal{F}(D(g_i))$. Using the positivity of H_i^2, and the fact that for the positive operators $A, B \geqslant 0$, their sum is positive also, with $\mathcal{N}(A + B) = \mathcal{N}(A) \cap \mathcal{N}(B)$, one finds

$$\mathcal{F}(G(D)) = \mathcal{N}\left(\sum_{i=1}^n H_i^2\right) \qquad \text{i.e.} \qquad G(D) = \lim_{t\to\infty} e^{-t\sum_{i=1}^n H_i^2}.$$

This means that instead of calculating all the projectors, one should find the operator $\sum_{i=1}^n H_i^2$, and the space $R = \mathcal{F}(G(D))$ of the fixed points is exactly the null-space of this operator.

It may be important to point out that the whole procedure also refers to the real representations, for which the standard reduction methods are not suitable. If a real representation $D(G)$ is to be decomposed onto its real (or physical) irreducible components $D^{(\mu)}(G)$, then the projector $G(D^{(\mu)} \otimes D)$ can be found by the proposed technique. Its trace is equal to the frequency number of $D^{(\mu)}(G)$ in $D(G)$, and the standard basis can be obtained exactly as has been described in the complex case.

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References

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