A Symmetry-Based Decomposition Approach to Eigenvalue Problems

Jun Fang · Xingyu Gao · Aihui Zhou

Abstract In this paper, we propose a decomposition approach to differential eigenvalue problems with Abelian or non-Abelian symmetries. In the approach, we divide the original differential problem into eigenvalue subproblems which require less eigenpairs and can be solved independently. Our approach can be seamlessly incorporated with grid-based discretizations such as finite difference, finite element, or finite volume methods. We place the approach into a two-level parallelization setting, which saves the CPU time remarkably. For illustration and application, we implement our approach with finite elements and carry out electronic structure calculations of some symmetric cluster systems, in which we solve thousands of eigenpairs with millions of degrees of freedom and demonstrate the effectiveness of the approach.

Keywords Eigenvalue · Grid-based discretization · Symmetry · Group theory · Two-level parallelism

Mathematics Subject Classification (2000) 65N25 · 65N30 · 65N05 · 81Q05

This work was partially supported by the National Science Foundation of China under Grant 61170310, the Funds for Creative Research Groups of China under Grant 11021101, the National Basic Research Program of China under Grants 2011CB309702 and 2011CB309703, and the National Center for Mathematics and Interdisciplinary Sciences, Chinese Academy of Sciences.

J. Fang · A. Zhou (✉)
LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China
e-mail: azhou@lsec.cc.ac.cn

J. Fang
e-mail: fangjun@lsec.cc.ac.cn

X. Gao
HPCC, Institute of Applied Physics and Computational Mathematics, Beijing 100094, China
e-mail: gao_xingyu@iapcm.ac.cn
Developing efficient numerical methods for eigenvalue problems are increasingly significant in modern scientific and engineering computing. We understand that a lot of eigenpairs have to be computed for instance when the size of the cluster system is large in electronic structure study, or the frequency range of interest is increased in structural analysis. To obtain accurate approximations, we see that a large number of degrees of freedom should be employed in discretizations. Since the computational cost of standard eigenvalue algorithms grows in proportion to $N_e^2 N$, where $N_e$ is the number of required eigenpairs and $N$ the number of degrees of freedom, we should decompose eigenvalue problems over degrees of freedom or over required eigenpairs. However, it is not easy to decompose an eigenvalue problem because the problem has an intrinsic nonlinearity and is set as a global optimization problem with orthonormal constraints. We observe that the existing efficient domain decomposition methods for boundary value problems usually do not work well for eigenvalue problems.

For an eigenvalue problem with symmetry, we are happy to see that the symmetry provides a way to do decomposition. As a systematic tool to study symmetry, group theory indicates that the eigenspace can be decomposed into orthogonal subspaces bearing distinct symmetry characteristics [8,9,34]. However, there are practical difficulties in using symmetry [3,39]. In quantum physics and quantum chemistry, people use the so-called symmetry-adapted bases to expand eigenfunctions in such orthogonal subspaces [8,9]. The symmetry-adapted bases are constructed from specific basis functions like atomic orbitals or internal coordinates of a molecule. A case-by-case illustration of the way to construct these bases from atomic orbitals has been given in [9], from which we see that the construction of symmetry-adapted bases is not an easy task. Later advances made in the application of group theory in structural mechanics adopt the idea of this classical approach, see review [43] and references cited therein.

We note that grid-based discretizations, such as finite difference, finite element, or finite volume methods, are widely used in scientific and engineering computing. For instance, the finite element method is often used to discretize eigenvalue problems in structural mechanics, see monograph [42], and grid-based discretization methods have been successfully applied to quantum eigenvalue problems in the last two decades, see [4,7,10,31,35] and references cited therein. Grid-based discretizations usually come with a large number of degrees of freedom. To construct symmetry-adapted bases would be a tedious process. Moreover, it will diminish the locality in grid-based discretizations and affect the customary procedure to form the matrix problem. Finite difference methods even do not have any basis function in the classical sense. These facts make it unfavorable to use symmetry-adapted bases with grid-based discretizations and large-scale ones in particular. Indeed, “the lack of general group-theoretic finite element programmes, noted by Wohlever [39] almost a decade ago, is still as true today as it was then” [43].

We propose a decomposition approach to differential eigenvalue problems with spatial symmetries, instead of using symmetry-adapted bases. In this approach, we decompose the original differential problem into eigenvalue subproblems. These subproblems share the original differential eigenvalue equation but are characterized by distinct symmetry conditions derived from group theory. Our approach can be seamlessly incorporated with grid-based discretizations and handle correctly the coupled subproblems encountered in the case of non-Abelian groups. Although we do not use symmetry-adapted bases, we provide a construction procedure for them, and then obtain theoretically the exact relation between approximate eigenpairs from our approach and those from using symmetry-adapted bases.
Since subproblems corresponding to different irreducible representations are decoupled, we may implement our approach using two-level parallelization, including a fundamental level of spatial parallelization and another level of subproblem distribution. For illustration, we use finite element discretizations, while the implementation techniques can be adapted to finite difference or finite volume methods, too. Due to the significance of first-principles calculations in quantum chemistry and materials science, we apply our approach to solving the Kohn–Sham equations of some symmetric cluster systems. Without the scale limit emphasized in [39], our approach has been effectively used to compute thousands of Kohn–Sham eigenstates with millions of degrees of freedom. We should mention that the decomposition of partial differential equations has also been exploited in [5, 6], which mainly focused on boundary value problems and did not provide any numerical result. We also see that symmetry has been utilized to simplify the solving of Kohn–Sham equations in a finite difference code [23]. However, they only handled Abelian groups there.

Both performance analysis and numerical tests indicate that our approach can reduce the CPU time remarkably, and would be attractive for large-scale eigenvalue problems. The computational overhead and memory requirement are reduced since each subproblem requires only a smaller number of eigenpairs, and we only need to store and compute part of the degrees of freedom due to the symmetry characteristics. Also, our two-level parallelization leads to a saving in the communication cost. Here we give an example to have a glance at the effectiveness of the approach. Consider the eigenvalue problem for the Laplacian in domain $(-1, 1)^3$ with zero boundary condition, and solve the first 1,000 smallest eigenvalues and associated eigenfunctions. We decompose the eigenvalue problem into 8 decoupled eigenvalue subproblems by applying Abelian group $D_{2h}$ which has 8 symmetry operations. The number of computed eigenpairs for each subproblem is 155, and the number of degrees of freedom for solving each subproblem, 205,379, is one eighth of that for the original problem, 1,643,032. We obtain a speedup of 28.8 by solving 8 subproblems instead of the original problem.

The rest of this paper is organized as follows. In Sect. 2, we propose our decomposition formulation based on group representation theory. Then in Sect. 3, we formulate matrix eigenvalue subproblems with general grid-based discretizations, and provide a construction procedure for symmetry-adapted bases, from which we obtain the exact relation between approximate eigenpairs from our approach and those from using symmetry-adapted bases. We quantitize the decrease in computational cost from our approach in Sect. 4, and address in Sect. 5 some critical implementation issues, including the two-level parallelization in particular. In Sect. 6, we validate our approach on a model eigenvalue problem for Abelian and non-Abelian symmetry groups, and show the reduction in computational and communication overhead. Then we apply the approach to solving the Kohn–Sham equations of symmetric clusters, in which we show that our approach can reduce the CPU time remarkably and would be attractive for large-scale eigenvalue problems. Finally, we give some concluding remarks.

2 Decomposition Formulation

In this section, we recall several basic but useful results of group theory and propose a symmetry-based decomposition formulation. The formulation, summarized as Theorem 1 and Corollary 2, can handle eigenvalue problems with Abelian or non-Abelian symmetries. Some notation and concepts will be given in Appendix 1.
2.1 Representation, Basis Function, and Projection Operator

We start from orthogonal coordinate transformations in $\mathbb{R}^d$ ($d = 1, 2, 3$) such as a rotation, a reflection or an inversion, that form a finite group $G$ of order $g$. Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and $V \subset L^2(\Omega)$ a Hilbert space of functions on $\Omega$ equipped with the $L^2$ scalar product $(\cdot, \cdot)$. Each $R \in G$ corresponds to an operator $P_R$ on $f \in V$ as

$$P_R f(Rx) = f(x) \quad \forall x \in \Omega.$$ 

It is proved that $\{P_R : R \in G\}$ form a group isomorphic to $G$.

A matrix representation of group $G$ means a group of matrices which is homomorphic to $G$. Any matrix representation with nonzero determinants is equivalent to a representation by unitary matrices (referred to as unitary representation). In the following we focus on unitary representations of group $G$.

The great orthogonality theorem (cf. [8, 9, 34]) tells that, all the inequivalent, irreducible, unitary representations $\{\Gamma^{(v)}\}$ of group $G$ satisfy

$$\sum_{R \in G} \Gamma^{(v)}(R)_{ml}^* \Gamma^{(v')}(R)_{m'l'} = \delta_{vv'} \delta_{mm'} \delta_{ll'} \frac{g}{d_v} \quad (1)$$

for any $l, m \in \{1, 2, \ldots, d_v\}$ and $l', m' \in \{1, 2, \ldots, d_{v'}\}$, where $d_v$ denotes the dimensionality of the $v$th representation $\Gamma^{(v)}$ and $\Gamma^{(v)}(R)_{ml}^*$ is the complex conjugate of $\Gamma^{(v)}(R)_{ml}$. The number of all the inequivalent, irreducible, unitary representations is equal to the number of classes in $G$. We denote this number as $n_c$.

**Definition 1** Given $v \in \{1, 2, \ldots, n_c\}$, non-zero functions $\{\phi_l^{(v)} : l = 1, 2, \ldots, d_v\} \subset V$ are said to form a basis for $\Gamma^{(v)}$ if for any $l \in \{1, 2, \ldots, d_v\}$

$$P_R \phi_l^{(v)} = \sum_{m=1}^{d_v} \phi_m^{(v)} \Gamma^{(v)}(R)_{ml} \quad \forall R \in G. \quad (2)$$

Function $\phi_l^{(v)}$ is called to belong to the $l$th column of $\Gamma^{(v)}$ (or adapt to the $v$-$l$ symmetry), and $\{\phi_m^{(v)} : m = 1, 2, \ldots, d_v, m \neq l\}$ are its partners.

There holds an orthogonality property for the basis functions (cf. [8, 9, 34]): if $\{\phi_l^{(v)} : l = 1, 2, \ldots, d_v\}$ and $\{\psi_{l'}^{(v')} : l' = 1, 2, \ldots, d_{v'}\}$ are basis functions for irreducible representations $\Gamma^{(v)}$ and $\Gamma^{(v')}$, respectively, then

$$(\phi_l^{(v)}, \psi_{l'}^{(v')}) = \delta_{vv'} \delta_{ll'} d_v^{-1} \sum_{m=1}^{d_v} (\phi_m^{(v)}, \psi_m^{(v)}) \quad (3)$$

holds for any $l \in \{1, 2, \ldots, d_v\}$ and $l' \in \{1, 2, \ldots, d_{v'}\}$. This equation implies that, two functions are orthogonal if they belong to different irreducible representations or to different columns of the same unitary representation. And the scalar product of two functions belonging to the same column of a given unitary representation (or adapting to the same symmetry) is independent of the column label.

Multiplying Eq. (2) by $\Gamma^{(v)}(R)_{m'l'}^*$ and summing over $R$, the great orthogonality theorem (1) implies that for any $l', m' \in \{1, 2, \ldots, d_{v'}\}$ and $l \in \{1, 2, \ldots, d_v\}$

$$\sum_{R \in G} \Gamma^{(v)}(R)_{m'l'}^* P_R \phi_l^{(v)} = \delta_{vv'} \delta_{ll'} \frac{g}{d_v} \phi_{m'}^{(v)}. \quad (4)$$

$\text{Springer}$
Define for any \( v \in \{1, 2, \ldots, n_c\} \) and \( l, m \in \{1, 2, \ldots, d_v\} \) operator \( \mathcal{D}_{ml}^{(v)} \) as

\[
\mathcal{D}_{ml}^{(v)} = \frac{d_v}{g} \sum_{R \in G} \Gamma^{(v)}(R)_{ml} P_R,
\]

we get

\[
\mathcal{D}_{ml}^{(v)} \phi_l^{(v')} = \delta_{v'v} \delta_{ll'} \phi_m^{(v)}
\]

for any \( v, v' \in \{1, 2, \ldots, n_c\}, l, m \in \{1, 2, \ldots, d_v\} \), and \( l' \in \{1, 2, \ldots, d_{v'}\} \).

**Proposition 1** Given \( v \in \{1, 2, \ldots, n_c\} \) and \( k \in \{1, 2, \ldots, d_v\} \). If \( v \in V \) satisfies \( \mathcal{D}_{kk}^{(v)} v \neq 0 \), then \( \{ \mathcal{D}_{kk}^{(v)} v : l = 1, 2, \ldots, d_v\} \) form a basis for \( \Gamma^{(v)} \), i.e., \( \{ \mathcal{D}_{kk}^{(v)} v : l = 1, 2, \ldots, d_v\} \) are non-zero functions, and for any \( l \in \{1, 2, \ldots, d_v\} \)

\[
P_R \left( \mathcal{D}_{lk}^{(v)} v \right) = \sum_{m=1}^{d_v} \left( \mathcal{D}_{mk}^{(v)} v \right) \Gamma^{(v)}(R)_{ml} \quad \forall R \in G.
\]

**Proof** For any \( l \in \{1, 2, \ldots, d_v\} \), we obtain from (4) that

\[
P_R \left( \mathcal{D}_{lk}^{(v)} v \right) = \frac{d_v}{g} \sum_{S \in G} \Gamma^{(v)}(S)_{lk} P_R S v = \frac{d_v}{g} \sum_{S' \in G} \Gamma^{(v)}(R^{-1}S')_{lk} P_S v \quad \forall R \in G,
\]

where \( P_R P_S = P_{RS} \) because \( \{ P_R : R \in G \} \) form a group isomorphic to \( G \).

Since \( \Gamma^{(v)} \) is a unitary representation of \( G \), we have

\[
P_R \left( \mathcal{D}_{lk}^{(v)} v \right) = \frac{d_v}{g} \sum_{S' \in G} \left( \sum_{m=1}^{d_v} \Gamma^{(v)}(R)_{ml} \Gamma^{(v)}(S')_{mk} \right) P_{S'} v,
\]

or

\[
P_R \left( \mathcal{D}_{lk}^{(v)} v \right) = \sum_{m=1}^{d_v} \left( \mathcal{D}_{mk}^{(v)} v \right) \Gamma^{(v)}(R)_{ml} \quad \forall R \in G.
\]

Recall the way to achieve (5), we see from the above equation and the great orthogonality theorem that

\[
\mathcal{D}_{kk}^{(v)} v = \mathcal{D}_{kl}^{(v)} \left( \mathcal{D}_{lk}^{(v)} v \right) \quad \forall l \in \{1, 2, \ldots, d_v\}.
\]

So \( \mathcal{D}_{kk}^{(v)} v \neq 0 \) indicates \( \mathcal{D}_{lk}^{(v)} v \neq 0 \) for all \( l \in \{1, 2, \ldots, d_v\} \). This completes the proof.

If we set \( v' = v, l' = l \) and \( m = l \) in (5), then we have for any \( v \in \{1, 2, \ldots, n_c\} \)

\[
\mathcal{D}_{ll}^{(v)} \phi_l^{(v)} = \phi_l^{(v)} \quad \forall l \in \{1, 2, \ldots, d_v\}.
\]

Proposition 1 implies that (6) serves to characterize the labels of any basis function:

**Corollary 1** Given \( v \in \{1, 2, \ldots, n_c\} \) and \( l \in \{1, 2, \ldots, d_v\} \). Non-zero function \( v \in V \) belongs to the \( l \)th column of \( \Gamma^{(v)} \) (or adapts to the \( v \)-\( l \) symmetry) if and only if

\[
\mathcal{D}_{ll}^{(v)} v = v.
\]

We will use the following properties of operator \( \mathcal{D}_{ml}^{(v)} \), whose proof is given in Appendix 2.
Proposition 2 Let \( \nu, \nu' \in \{1, 2, \ldots, n_c\}, l, m \in \{1, 2, \ldots, d_\nu\}, \) and \( l', m' \in \{1, 2, \ldots, d_{\nu'}\} \).

(a) The adjoint of operator \( P_{ml}^{(\nu)} \) satisfies
\[
P_{ml}^{(\nu)*} = P_{lm}^{(\nu)}.
\]

(b) The multiplication of two operators \( P_{ml}^{(\nu)} \) and \( P_{m'l'}^{(\nu')} \) satisfies
\[
P_{ml}^{(\nu)} P_{m'l'}^{(\nu')} = \delta_{\nu \nu'} \delta_{lm} P_{ml}^{(\nu')}.
\]

2.2 Subproblems

We see from Corollary 1 and the linearity of operator \( P_{ll}^{(\nu)} \) that, all functions in \( V \) belonging to the \( l \)th column of \( \Gamma^{(\nu)} \) (or adapting to the \( \nu \)-\( l \) symmetry) form a subspace of \( V \). We denote this subspace by \( V_l^{(\nu)} \).

There holds a decomposition theorem for any function in \( V \) (cf. [8, 9, 34]): any \( f \in V \) can be decomposed into a sum of the form
\[
f = \sum_{\nu=1}^{n_c} \sum_{l=1}^{d_\nu} f_l^{(\nu)},
\]
where \( f_l^{(\nu)} \in V_l^{(\nu)} \). We see from (5) and (7) that \( P_{ll}^{(\nu)} : V \rightarrow V_l^{(\nu)} \) is a projection operator. Equation (7) implies
\[
V = \sum_{\nu=1}^{n_c} \sum_{l=1}^{d_\nu} V_l^{(\nu)},
\]
which indeed is a direct sum
\[
V = \bigoplus_{\nu=1}^{n_c} \bigoplus_{l=1}^{d_\nu} V_l^{(\nu)}
\]
due to (3).

Now we turn to study the symmetry-based decomposition for eigenvalue problems. Consider eigenvalue problems of the form
\[
Lu = \lambda u \quad \text{in} \ \Omega
\]
subject to some boundary condition, where \( L \) is an Hermitian operator. Group \( G \) is said to be a symmetry group associated with eigenvalue problem (9) if
\[
R \Omega = \Omega, \quad P_R L = L P_R \quad \forall R \in G,
\]
and the subjected boundary condition is also invariant under \( \{P_R\} \). Then any \( R \in G \) is called a symmetry operation for problem (9). For simplicity, we take zero boundary condition as an example and discuss the decomposition of eigenvalue problem
\[
\begin{cases}
Lu = \lambda u \quad \text{in} \ \Omega, \\
u = 0 \quad \text{on} \ \partial \Omega.
\end{cases}
\]

Since \( P_R \) and \( L \) are commutative for any \( R \) in \( G \), we have:

Proposition 3 If \( \nu \in V_l^{(\nu)} \), then \( L \nu \in V_l^{(\nu)} \), where \( \nu \in \{1, 2, \ldots, n_c\} \) and \( l \in \{1, 2, \ldots, d_\nu\} \). In other words, \( V_l^{(\nu)} \) is an invariant subspace of operator \( L \).
Due to the direct sum decomposition of space \( V \) and Proposition 3, we obtain a decomposition of the eigenvalue problem as follows:

**Theorem 1** Suppose finite group \( G = \{ R \} \) is a symmetry group associated with eigenvalue problem (10). Denote all the inequivalent, irreducible, unitary representations of \( G \) as \( \{ \Gamma_v : v = 1, 2, \ldots, n_c \} \). Then the eigenvalue problem can be decomposed into \( \sum_{v=1}^{n_c} d_v \) subproblems. For any \( v \in \{ 1, 2, \ldots, n_c \} \), the corresponding \( d_v \) subproblems are

\[
\begin{aligned}
& L_{l_1}^{(v)} u^{(v)}_{l_1} = \lambda^{(v)}_{l_1} u^{(v)}_{l_1} & \quad & \text{in } \Omega, \\
& u^{(v)}_{l_1} = 0 & \quad & \text{on } \partial \Omega, \quad l = 1, 2, \ldots, d_v, \\
& u^{(v)}_{l_1} = \mathcal{P}_{l_k}^{(v)} u^{(v)}_{k} & \quad & \text{in } \Omega,
\end{aligned}
\]

where \( k \) is any chosen number in \( \{ 1, 2, \ldots, d_v \} \).

**Proof** We see from (8) and Proposition 3 that, other than solving the eigenvalue problem in \( V \), we can solve the problem in each subspace \( V^{(v)}_l \) independently. More precisely, we can decompose the original eigenvalue problem (10) into \( \sum_{v=1}^{n_c} d_v \) subproblems; for any \( v \in \{ 1, 2, \ldots, n_c \} \), the \( d_v \) subproblems are as follows

\[
\begin{aligned}
& L_{l_1}^{(v)} u^{(v)}_{l_1} = \lambda^{(v)}_{l_1} u^{(v)}_{l_1} & \quad & \text{in } \Omega, \\
& u^{(v)}_{l_1} = 0 & \quad & \text{on } \partial \Omega, \quad l = 1, 2, \ldots, d_v, \\
& \mathcal{P}_{l_1}^{(v)} u^{(v)}_{l_1} = u^{(v)}_{l_1} & \quad & \text{in } \Omega,
\end{aligned}
\]

where the third equation characterizes \( u^{(v)}_{l_1} \in V^{(v)}_l \), as indicated in Corollary 1.

Given any \( v \in \{ 1, 2, \ldots, n_c \} \), we consider the \( d_v \) subproblems (12). We shall prove that, for any \( k, l \in \{ 1, 2, \ldots, d_v \} \), if \( v \) and \( w \) are two orthogonal eigenfunctions corresponding to some eigenvalue of the \( k \)th subproblem, then \( \mathcal{P}_{l_k}^{(v)} v \) and \( \mathcal{P}_{l_k}^{(v)} w \) are eigenfunctions of the \( l \)th subproblem with the same eigenvalue, and are also orthogonal.

Combining (5) and the fact that \( P_R \) and \( L \) are commutative for each \( R \), we obtain that \( \mathcal{P}_{l_k}^{(v)} v \) is an eigenfunction of the \( l \)th subproblem which corresponds to the same eigenvalue as the one for \( v \). It remains to prove the orthogonality of \( \mathcal{P}_{l_k}^{(v)} v \) and \( \mathcal{P}_{l_k}^{(v)} w \). Proposition 2 indicates that the scalar product of any two functions in \( V^{(v)}_k \) is invariant after operating on them with \( \mathcal{P}_{l_k}^{(v)} \). Indeed, we have for any \( v, w \in V^{(v)}_k \) that

\[
(\mathcal{P}_{l_k}^{(v)} v, \mathcal{P}_{l_k}^{(v)} w) = (\mathcal{P}_{l_k}^{(v)*} \mathcal{P}_{l_k}^{(v)} v, w) = (\mathcal{P}_{l_k}^{(v)} \mathcal{P}_{l_k}^{(v)} v, w) = (\mathcal{P}_{l_k}^{(v)} v, w),
\]

which together with Corollary 1 leads to

\[
(\mathcal{P}_{l_k}^{(v)} v, \mathcal{P}_{l_k}^{(v)} w) = (v, w).
\]

Thus \( \mathcal{P}_{l_k}^{(v)} v \) and \( \mathcal{P}_{l_k}^{(v)} w \) are orthogonal when \( v \) and \( w \) are.

Since \( L \) is Hermitian, we see that for the \( d_v \) subproblems (12), eigenvalues of the \( l \)th subproblem are the same as those of the \( k \)th one, and eigenfunctions of the \( l \)th subproblem can be chosen as \( \{ \mathcal{P}_{l_k}^{(v)} v \} \), where \( \{ v \} \) are eigenfunctions of the \( k \)th subproblem and \( k \) is any chosen number in \( \{ 1, 2, \ldots, d_v \} \).

Therefore, the original eigenvalue problem (10) is decomposed into \( \sum_{v=1}^{n_c} d_v \) subproblems, and for any \( v \in \{ 1, 2, \ldots, n_c \} \) the corresponding \( d_v \) subproblems can be given as (11). This completes the proof. \( \square \)
The third equation of the \( d_v \) subproblems in (11) are
\[
\begin{align*}
\nu_k^{(v)} &= \mathcal{P}_{kk}^{(v)} u_k^{(v)}, \\
\nu_l^{(v)} &= \mathcal{P}_{lk}^{(v)} u_k^{(v)} \quad \forall \ l = 1, 2, \ldots, d_v, \ l \neq k.
\end{align*}
\]
We see from Proposition 1 that \( \{\nu_l^{(v)} : l = 1, 2, \ldots, d_v\} \) form a basis for \( \Gamma^{(v)} \). Namely, for any \( l \in \{1, 2, \ldots, d_v\} \)
\[
P_R \nu_l^{(v)} = \sum_{m=1}^{d_v} \nu_m^{(v)} \Gamma(R)_{ml} \quad \forall R \in G,
\]
i.e.,
\[
\nu_l^{(v)}(Rx) = \sum_{m=1}^{d_v} \Gamma(R)_{ml} \nu_m^{(v)}(x) \quad \forall R \in G.
\]

**Corollary 2** Under the same condition as in Theorem 1, eigenvalue problem (10) can be decomposed into \( \sum_{v=1}^{n_c} d_v \) subproblems. For any \( v \in \{1, 2, \ldots, n_c\} \), the corresponding \( d_v \) subproblems can be given as follows
\[
\begin{align*}
L \nu_l^{(v)} &= \lambda^{(v)} \nu_l^{(v)} \quad \text{in} \ \Omega, \\
\nu_l^{(v)} &= 0 \quad \text{on} \ \partial \Omega, \\
\nu_l^{(v)}(Rx) &= \sum_{m=1}^{d_v} \Gamma(R)_{ml} \nu_m^{(v)}(x) \quad \text{in} \ \Omega, \ \forall R \in G.
\end{align*}
\]

The third equations in (11) and (13) describe symmetry properties of eigenfunctions over domain \( \Omega \). The original eigenvalue problem can be decomposed into subproblems just because eigenfunctions of subproblems satisfy distinct equations. In the following text, we call these equations as symmetry characteristics.

Denote by \( \Omega_0 \) the smallest subdomain which produces \( \Omega \) by applying all symmetry operations \( \{R \in G\} \), namely, \( \Omega = \bigcup_{R \in G} R\Omega_0 \), and \( R_1 \Omega_0 \cap R_2 \Omega_0 = \emptyset \) for any \( R_1, R_2 \in G \) satisfying \( R_1 \neq R_2 \). We call \( \Omega_0 \) the irreducible subdomain and the associated volume is \( g \) times smaller than that of \( \Omega \). The symmetry characteristic equation in (13) tells that for any \( l \in \{1, 2, \ldots, d_v\} \), \( \nu_l^{(v)} \) over \( \Omega \) is determined by the values of functions \( \{\nu_1^{(v)}, \ldots, \nu_{d_v}^{(v)}\} \) over \( \Omega_0 \).

**Remark 1** A decomposition formulation has been shown in [6] for boundary value problems with spatial symmetries. Each decomposed problem is defined on the irreducible subdomain \( \Omega_0 \) and characterized by a “boundary condition” on \( \Sigma \), which is in fact a restriction of the symmetry characteristic on \( \Sigma \). Indeed, symmetry characteristics over \( \Omega \) should not be replaced by the restriction on the internal boundary in general. In special cases, it is true that we can derive internal boundary conditions such as Dirichlet or Neumann type from the symmetry characteristics, and then define subproblems on \( \Omega_0 \). While in the deduction of Neumann boundary conditions one has to use the symmetry characteristic near the internal boundary, not only on the boundary.

---

1 In [6], \( \Sigma \) is the “internal” boundary \( \partial \Omega_0 \setminus \partial \Omega \) of \( \Omega_0 \), and irreducible subdomain \( \Omega_0 \) is called symmetry cell.
Under the assumption that all symmetries of the eigenvalue problem are included in group $G$ and no accidental degeneracy occurs, the eigenvalue degeneracy is determined by the dimensionalities of irreducible representations of $G$ $[8,9,34]$. For example, in cubic crystals $^2$ all eigenstates have degeneracy 1, 2, or 3 $[26]$. According to Theorem 1 or Corollary 2, eigenvalues of each subproblem should be nondegenerate. In practice, we usually use part of symmetry operations. Thus subproblems will probably still have degenerate eigenvalues. However, it is possible to improve the spectral separation, especially when we exploit as many symmetries as possible. This would benefit the convergence of iterative diagonalization.

In Appendix 3, we explain subproblem formulation (13) in Corollary 2 using a simple example. Formulation (13) makes a straightforward implementation with grid-based discretizations. We shall discuss the way to solve the subproblems in the next section.

3 Discretization

In this section, we study the matrix eigenvalue problems associated with subproblems (11) and (13). We formulate our matrix eigenvalue subproblems with general grid-based discretizations. Then we provide a construction procedure for symmetry-adapted bases, based on which we obtain the relation between approximate eigenpairs from our approach and those from using symmetry-adapted bases.

Note that subproblems associated with different $\nu$ values are independent and have the same formulation. So we take one $\nu \in \{1, 2, \ldots, n_c\}$ and discuss the corresponding $d_\nu$ subproblems.

3.1 Our discretized system

Suppose $\Omega$ is discretized by a symmetrical grid with respect to group $G$, and $N$ is the number of degrees of freedom. For simplicity we assume that no degree of freedom lies on symmetry elements.$^3$

We determine a smallest set of degrees of freedom that could produce all $N$ ones by applying symmetry operations $\{R \in G\}$. It is clear that the number of degrees of freedom in this smallest set satisfies $N_0 = N / g$. We denote the set as

$$\{x_j : j = 1, 2, \ldots, N_0\},$$

then all degrees of freedom can be given by

$$\{R(j) : j = 1, 2, \ldots, N_0, \ R \in G\},$$

where $R(j) \equiv Rx_j \ (j = 1, 2, \ldots, N_0)$.

The symmetry characteristic equation in (13) tells that for any $l \in \{1, 2, \ldots, d_\nu\}$, the values of $u^{(\nu)}_l$ on all degrees of freedom $\{R(j) : j = 1, 2, \ldots, N_0, \ R \in G\}$ are determined by the values of $\{u^{(\nu)}_1, \ldots, u^{(\nu)}_{d_\nu}\}$ on $\{j : j = 1, 2, \ldots, N_0\}$. Thus, the size of discretized eigenvalue problem for (13) is $d_\nu N_0$.

$^2$ Cubic crystals are crystals where the unit cell is a cube. All irreducible representations of the associated symmetry group are one-, two-, or three-dimensional.

$^3$ Symmetry element of operation $R$ is a point of reference about which $R$ is carried out, such as a point to do inversion, a rotation axis, or a reflection plane. Symmetry element is invariant under the associated symmetry operation.
If the given irreducible representation $\Gamma^{(v)}$ is one-dimensional, then (13) gives

\[
\begin{aligned}
\begin{cases}
Lu^{(v)} = \lambda^{(v)}u^{(v)} & \text{in } \Omega,
\end{cases}
\end{aligned}
\]

\[
\begin{aligned}
\begin{cases}
u^{(v)} = 0 & \text{on } \partial \Omega,
\end{cases}
\end{aligned}
\]

\[
\begin{aligned}
\begin{cases}
u^{(v)}(Rx) = \Gamma^{(v)}(R)_{\ast}u^{(v)}(x) & \text{in } \Omega, \ \forall R \in G,
\end{cases}
\end{aligned}
\]

where we omit subscripts of $\Gamma^{(v)}(R)_{\ast}$ and $u^{(v)}_{1}$.

Suppose the discretized system for eigenvalue problem (14) is

\[
\begin{aligned}
\begin{cases}
\sum_{j=1}^{N_{0}} \sum_{R \in G} a_{i,R(j)}u_{R(j)} = \lambda \sum_{j=1}^{N_{0}} \sum_{R \in G} b_{i,R(j)}u_{R(j)}, & i = 1, 2, \ldots, N_{0},
\end{cases}
\end{aligned}
\]

where $u_{R(j)}$ is the unknown associated with $Rx_{j}$ and $\{a_{i,R(j)}, b_{i,R(j)}\}$ represent the discretization coefficients. For instance, in finite element discretizations, $a_{i,R(j)}$ and $b_{i,R(j)}$ are entries of the stiffness and mass matrices, respectively. Note that for any $i \in \{1, 2, \ldots, N_{0}\}$, although the discretization equation seems to involve all $N$ degrees of freedom $\{R(j) : j = 1, 2, \ldots, N_{0}, R \in G\}$, in fact only part of coefficients $\{a_{i,R(j)}, b_{i,R(j)} : j = 1, 2, \ldots, N_{0}, R \in G\}$ are non-zero. An extreme example is that in finite difference discretizations $b_{i,R(j)} = \delta_{i,R(j)}$ ($j = 1, 2, \ldots, N_{0}, R \in G$) for any $i \in \{1, 2, \ldots, N_{0}\}$.

We know from the symmetry characteristic equation that the discretized system is then reduced to

\[
\sum_{j=1}^{N_{0}} \sum_{R \in G} \Gamma^{(v)}(R)_{\ast} a_{i,R(j)} u_{j} = \lambda \sum_{j=1}^{N_{0}} \sum_{R \in G} \Gamma^{(v)}(R)_{\ast} b_{i,R(j)} u_{j}, \quad i = 1, 2, \ldots, N_{0}.
\]

Denote the solution vector as

\[
u = (u_{1}, u_{2}, \ldots, u_{N_{0}})^{T},
\]

we may rewrite the discretized system as a matrix form

\[
Au = \lambda Bu,
\]

where

\[
A = (A_{ij})_{N_{0} \times N_{0}}, \quad A_{ij} = \sum_{R \in G} \Gamma^{(v)}(R)_{\ast} a_{i,R(j)},
\]

\[
B = (B_{ij})_{N_{0} \times N_{0}}, \quad B_{ij} = \sum_{R \in G} \Gamma^{(v)}(R)_{\ast} b_{i,R(j)}.
\]

(15)

In the case of higher-dimensional irreducible representations, the $d_{\nu}$ subproblems in (13) are coupled through symmetry characteristics. Taking $d_{\nu} = 2$ as an example, we assemble subproblems for $u^{(v)}_{1}$ and $u^{(v)}_{2}$ in (13) to solve eigenvalue problem

\[
\begin{aligned}
\begin{cases}
Lu^{(v)}_{1} = \lambda^{(v)} u^{(v)}_{1} & \text{in } \Omega,
\end{cases}
\end{aligned}
\]

\[
\begin{aligned}
\begin{cases}
u^{(v)} = 0 & \text{on } \partial \Omega,
\end{cases}
\end{aligned}
\]

\[
\begin{aligned}
\begin{cases}
u^{(v)}(Rx) = \Gamma^{(v)}(R)_{11}^{\ast} u^{(v)}_{1} + \Gamma^{(v)}(R)_{12}^{\ast} u^{(v)}_{2} & \text{in } \Omega, \ \forall R \in G,
\end{cases}
\end{aligned}
\]

\[
\begin{aligned}
\begin{cases}
u^{(v)}(Rx) = \Gamma^{(v)}(R)_{21}^{\ast} u^{(v)}_{1} + \Gamma^{(v)}(R)_{22}^{\ast} u^{(v)}_{2} & \text{in } \Omega, \ \forall R \in G,
\end{cases}
\end{aligned}
\]

\[
\begin{aligned}
\begin{cases}
u^{(v)} = 0 & \text{on } \partial \Omega.
\end{cases}
\end{aligned}
\]
Suppose the discretized system associated with (16) is
\[
\begin{align*}
    &\sum_{j=1}^{N_0} \sum_{R \in G} a_{i,R(j)} u_{1,R(j)} = \lambda \sum_{j=1}^{N_0} \sum_{R \in G} b_{i,R(j)} u_{1,R(j)}, & i = 1, 2, \ldots, N_0, \\
    &\sum_{j=1}^{N_0} \sum_{R \in G} a_{i,R(j)} u_{2,R(j)} = \lambda \sum_{j=1}^{N_0} \sum_{R \in G} b_{i,R(j)} u_{2,R(j)}, & i = 1, 2, \ldots, N_0,
\end{align*}
\]
where \(u_{1,R(j)}\) and \(u_{2,R(j)}\) are the unknowns associated with \(Rx_j\). Denote the solution vector as
\[
    \mathbf{v} = (u_{11}, u_{12}, \ldots, u_{1N_0}, u_{21}, u_{22}, \ldots, u_{2N_0})^T
\]
and rewrite the discretized system as a matrix form
\[
    A\mathbf{v} = \lambda B\mathbf{v}. \tag{17}
\]
We have
\[
    A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix},
\]
where \(A_{ml} = (A_{ml})_{N_0 \times N_0}\) \((m, l = 1, 2)\) with
\[
    A_{11} = \sum_{R \in G} \Gamma^{(v)}(R)_{11}^* a_{i,R(j)}, \quad A_{12} = \sum_{R \in G} \Gamma^{(v)}(R)_{12}^* a_{i,R(j)}, \\
    A_{21} = \sum_{R \in G} \Gamma^{(v)}(R)_{21}^* a_{i,R(j)}, \quad A_{22} = \sum_{R \in G} \Gamma^{(v)}(R)_{22}^* a_{i,R(j)}.
\]
Entries of \(B\) are in the same form as those of \(A\) and can be obtained by substituting \(a_{i,R(j)}\) with \(b_{i,R(j)}\).

If symmetry group \(G\) is Abelian, each irreducible representation is one-dimensional and all discretized subproblems are independent. Otherwise, there exist \(\Gamma^{(v)}(\cdot)\) with \(d_v > 1\) and the corresponding \(d_v\) discretized subproblems are coupled through symmetry characteristics. Thus, no matter \(G\) is Abelian or not, we shall solve \(n_c\) decoupled matrix eigenvalue problems, and the size of the \(v\)th one is \(d_v N_0\).

### 3.2 Symmetry-Adapted Bases

In Sect. 3.3, we shall obtain the relation between approximate eigenpairs from our approach and the approach which uses symmetry-adapted bases. For this purpose, in the current subsection, we provide a construction procedure for the symmetry-adapted bases, which is the most critical step in the latter approach.

Consider the weak form of (10): find \((\lambda, u) \in \mathbb{R} \times V\) such that
\[
a(u, v) = \lambda (u, v) \quad \forall v \in V,
\]
where \(a(\cdot, \cdot)\) is the associated bilinear form over \(V \times V\).

Note that the discussion in this part is not restricted to grid-based discretizations, but we still use notation \(N\) and \(N_0\) for brevity. Suppose that we start from \(N\) basis functions \(\{\psi\}\) of some type, which satisfy that for any \(R \in G\), \(P_R \psi\) is one of the basis functions when \(\psi\) is, i.e., the \(N\) basis functions are chosen with respect to symmetry group \(G\). For simplicity, like the assumption for grid-based discretizations, we assume that the \(g\) basis functions \(\{P_R \psi : R \in G\}\) are linearly independent for any basis function \(\psi\). We see that the
number of basis functions in the set which could produce all $N$ ones by applying $\{R \in G\}$ is $g$ times smaller than $N$. We denote this set by

$$\{\psi_j : j = 1, 2, \ldots, N\},$$

then all basis functions are given as

$$\{P_R \psi_j : j = 1, 2, \ldots, N, \ R \in G\}.$$

For the given $\nu$, we fix some $k \in \{1, 2, \ldots, d_{\nu}\}$ and generate symmetry-adapted bases for the $k$th subproblem in (11). This is achieved by applying projection operator $\mathcal{S}_{kk}^{(\nu)}$ on all the basis functions $\{P_R \psi_j : j = 1, 2, \ldots, N, \ R \in G\}$. Suppose that we obtain $N'$ linearly independent symmetry-adapted bases from this process and we denote them as $\{\psi_j : j = 1, 2, \ldots, N'\}$. Then for any $l \in \{1, 2, \ldots, d_{\nu}\}$, we generate symmetry-adapted bases for the $l$th subproblem as $\{\mathcal{S}_{lk}^{(\nu)} \psi_j : j = 1, 2, \ldots, N'\}$.

Consider the $d_{\nu}$ matrix subproblems under the generated symmetry-adapted bases for (11). They are decoupled eigenvalue problems and matrix elements of the $l$th problem are

$$a(\mathcal{S}_{lk}^{(\nu)} \psi_j, \mathcal{S}_{lk}^{(\nu)} \psi_l), \ (\mathcal{S}_{lk}^{(\nu)} \psi_j, \mathcal{S}_{lk}^{(\nu)} \psi_l), \ i, j = 1, 2, \ldots, N'.$$

For each $j \in \{1, 2, \ldots, N'\}$, according to Proposition 1, $\{\mathcal{S}_{lk}^{(\nu)} \psi_l : l = 1, 2, \ldots, d_{\nu}\}$ form a basis for $\Gamma^{(\nu)}$. We see from (3) and Proposition 3 that all the $d_{\nu}$ matrix eigenvalue problems are the same. So we only need to solve the one corresponding to the $k$th subproblem:

$$\sum_{j=1}^{N'} a(\psi_j, \psi_l) \alpha_j = \lambda^{(\nu)} \sum_{j=1}^{N'} (\psi_j, \psi_l) \alpha_j, \ i = 1, 2, \ldots, N',$$

where $\{\alpha_j\}$ are the unknowns. After calculating $\{\alpha_j\}$, the approximated eigenfunctions for the $l$th subproblem can be achieved by

$$u_l^{(\nu)} = \sum_{j=1}^{N'} \alpha_j \mathcal{S}_{lk}^{(\nu)} \psi_j, \ l = 1, 2, \ldots, d_{\nu}.$$

Next we show how many symmetry-adapted bases would be constructed for the $v$-$k$ symmetry, i.e., the number $N'$ of linearly independent symmetry-adapted functions in

$$\mathcal{S}_{kk}^{(\nu)} \{P_R \psi_j : j = 1, 2, \ldots, N, \ R \in G\}.$$

And then we give the specific way to obtain these functions.

**Theorem 2** Suppose the original basis functions $\{P_R \psi_j : j = 1, 2, \ldots, N, \ R \in G\}$ satisfy that for each $j \in \{1, 2, \ldots, N\}$ the $g$ functions in $\{P_R \psi_j : R \in G\}$ are linearly independent. Then for any given $v \in \{1, 2, \ldots, n_c\}$ and $k \in \{1, 2, \ldots, d_{\nu}\}$, there are $d_{\nu} N$ symmetry-adapted bases for the $v$-$k$ symmetry.

**Proof** We need to prove that there are exactly $d_{\nu} N$ linearly independent symmetry-adapted functions in $\{\mathcal{S}_{kk}^{(\nu)} P_R \psi_j : j = 1, 2, \ldots, N, \ R \in G\}$.

For any $R \in G$ and $j \in \{1, 2, \ldots, N\}$, since

$$\mathcal{S}_{kk}^{(\nu)} P_R \psi_j = \frac{d_{\nu}}{g} \sum_{R' \in G} \Gamma^{(\nu)} (R')_{kk}^* P_R' P_R \psi_j = \frac{d_{\nu}}{g} \sum_{S \in G} \Gamma^{(\nu)} (SR^{-1})_{kk}^* P_S \psi_j, \quad (18)$$
we see that $\mathcal{P}_{kk}^{(v)} P_R \psi_j$ is a linear combination of functions $\{P_S \psi_j : S \in G\}$ and the coefficient of $P_S \psi_j$ is $\frac{\partial}{\partial x} \Gamma^{(v)}(SR^{-1})_{kk}^*$, Obviously, functions in $\{\mathcal{P}_{kk}^{(v)} P_R \psi_j : j = 1, 2, \ldots, N_0, \ R \in G\}$ with different $j$ values are linearly independent. So we only need to determine the number of symmetry-adapted bases in $\{\mathcal{P}_{kk}^{(v)} P_R \psi_j : R \in G\}$ for any given $j \in \{1, 2, \ldots, N_0\}$.

Since $\{P_S \psi_j : S \in G\}$ are linearly independent and $R^{-1}$ runs over all elements of group $G$ when $R$ does, (18) tells that the number of linearly independent functions in $\{\mathcal{P}_{kk}^{(v)} P_R \psi_j : R \in G\}$ equals to the rank of matrix $C = (C_{mn})_{g \times g}$, where $C_{mn} = \Gamma^{(v)}(R_m R_n)_{kk}$.

We observe that $C$ can be written as

$$
C = \begin{bmatrix}
\Gamma^{(v)}(R_1)_{1k}^* & \ldots & \Gamma^{(v)}(R_1)_{dk}^* \\
\Gamma^{(v)}(R_2)_{1k}^* & \ldots & \Gamma^{(v)}(R_2)_{dk}^* \\
\vdots & \ddots & \vdots \\
\Gamma^{(v)}(R_g)_{1k}^* & \ldots & \Gamma^{(v)}(R_g)_{dk}^*
\end{bmatrix}
\begin{bmatrix}
\Gamma^{(v)}(R_1)_{1k}^* & \ldots & \Gamma^{(v)}(R_g)_{1k}^* \\
\Gamma^{(v)}(R_1)_{2k}^* & \ldots & \Gamma^{(v)}(R_g)_{2k}^* \\
\vdots & \ddots & \vdots \\
\Gamma^{(v)}(R_1)_{d_k,k}^* & \ldots & \Gamma^{(v)}(R_g)_{d_k,k}^*
\end{bmatrix} = C_1 C_2,
$$

where $C_1$ and $C_2$ are $g \times d_v$ and $d_v \times g$ matrices, respectively. We obtain from the great orthogonality theorem (1) that columns of $C_1$ are orthogonal, and so are rows of $C_2$, i.e.,

$$\text{rank}(C_1) = \text{rank}(C_2) = d_v.$$

Thus

$$\text{rank}(C) = \text{rank}(C_1 C_2) = d_v,$$

and we completed the proof. \hfill \Box

Remark 2 For the given $v$ and $k$, Theorem 2 indicates that there are $d_v$ symmetry-adapted bases for each $j \in \{1, 2, \ldots, N_0\}$. It remains a problem how to obtain these $d_v$ functions. We see from (18) that, whenever the chosen $d_v$ operations $\{R_n \in G : n = 1, 2, \ldots, d_v\}$ satisfy that the $k$th columns of matrices $\{\Gamma^{(v)}(R_n^{-1}) : n = 1, 2, \ldots, d_v\}$ are linearly independent, $\{\mathcal{P}_{kk}^{(v)} P_{R_n} \psi_j : n = 1, 2, \ldots, d_v\}$ exactly give the $d_v$ symmetry-adapted bases.

3.3 Relation

In this part, taking the finite element discretization as an example, we investigate the relation between approximate eigenpairs from our approach and those from the approach which uses symmetry-adapted bases.

Consider the finite element discretization and denote the basis function corresponding to any $j \in \{1, 2, \ldots, N_0\}$ as $\varphi_j$. We see from $P_R \varphi_j(x) = \varphi_j(R^{-1}x)$ that $P_R \varphi_j$ is the basis function corresponding to $R(j)$, i.e.,

$$P_R \varphi_j = \varphi_{R(j)}.$$

Our discretized systems associated with the finite element basis functions $\{P_R \varphi_j : j = 1, 2, \ldots, N_0, \ R \in G\}$ are determined by setting $a_{i,R(j)}$ and $b_{i,R(j)}$ in (15) and (17) as

$$a_{i,R(j)} = (P_R \varphi_j, \varphi_i), \quad b_{i,R(j)} = (P_R \varphi_j, \varphi_i).$$

Now we turn to study matrix eigenvalue problem for the approach which uses symmetry-adapted bases, and obtain the relation between the two approaches.

In the case of $d_v = 1$, we apply projection operator $\mathcal{P}^{(v)}$ on all the finite element basis functions to construct symmetry-adapted bases. We see from Theorem 2 that for each $j \in \{1, 2, \ldots, N_0\}$, $\{\mathcal{P}^{(v)} P_R \varphi_j : R \in G\}$ give just one symmetry-adapted basis function.
According to Remark 2, we can choose \( R = E \) to get all the \( N_0 \) symmetry-adapted bases as follows
\[
\Phi_j = \mathcal{P}^{(v)} \varphi_j, \quad j = 1, 2, \ldots, N_0.
\]

The matrix eigenvalue problem under these bases then becomes
\[
\sum_{j=1}^{N_0} a(\Phi_j, \Phi_j) c_j = \tilde{\lambda} \sum_{j=1}^{N_0} (\Phi_j, \Phi_i) c_j, \quad i = 1, 2, \ldots, N_0,
\]
where \( \{c_j\} \) are the unknowns. Equivalently,
\[
\tilde{A} \tilde{u} = \tilde{\lambda} \tilde{B} \tilde{u},
\]
where \( \tilde{u} = (c_1, c_2, \ldots, c_{N_0})^T \) and
\[
\begin{align*}
\tilde{A} &= (\tilde{A}_{ij})_{N_0 \times N_0}, \quad \tilde{A}_{ij} = \frac{1}{g} \sum_{R \in G} \Gamma^{(v)}(R)^* a(P_R \varphi_j, \varphi_i), \\
\tilde{B} &= (\tilde{B}_{ij})_{N_0 \times N_0}, \quad \tilde{B}_{ij} = \frac{1}{g} \sum_{R \in G} \Gamma^{(v)}(R)^* (P_R \varphi_j, \varphi_i).
\end{align*}
\]

Comparing (20) with matrices (15) in our approach and using (19), we obtain
\[
\begin{align*}
\tilde{A} &= \frac{1}{g} A, \quad \tilde{B} = \frac{1}{g} B.
\end{align*}
\]

Thus, in the case of \( d_v = 1 \), there holds
\[
\lambda = \tilde{\lambda}, \quad u = \tilde{u}.
\]

In the case of \( d_v = 2 \), there are two subproblems in (11). We choose \( k = 1 \) and apply projection operator \( \mathcal{P}^{(v)}_{11} \) on all the finite element basis functions to construct symmetry-adapted bases for the first subproblem. Theorem 2 tells that for each \( j \in \{1, 2, \ldots, N_0\} \), \( \{\mathcal{P}^{(v)}_{11} P_S \varphi_j : R \in G\} \) give \( d_v = 2 \) symmetry-adapted bases. According to Remark 2, we choose identity operation \( E \) and another \( S \in G \) which satisfy that the first columns of matrices \( \{\Gamma^{(v)}(E), \Gamma^{(v)}(S^{-1})\} \) are linearly independent. Then
\[
\{\mathcal{P}^{(v)}_{11} \varphi_j, \mathcal{P}^{(v)}_{11} P_S \varphi_j : j = 1, 2, \ldots, N_0\}
\]
give all the \( 2N_0 \) bases adapted to the \( v \)-1 symmetry as follows
\[
(\Phi_1, \ldots, \Phi_{N_0}, \Psi_1, \ldots, \Psi_{N_0}) = (\mathcal{P}^{(v)}_{11} \varphi_1, \ldots, \mathcal{P}^{(v)}_{11} \varphi_{N_0}, \mathcal{P}^{(v)}_{11} P_S \varphi_1, \ldots, \mathcal{P}^{(v)}_{11} P_S \varphi_{N_0}).
\]

The matrix eigenvalue problem under these bases is
\[
\begin{align*}
\sum_{j=1}^{N_0} a(c_{1j} \Phi_j + c_{2j} \Psi_j, \Phi_i) &= \lambda \sum_{j=1}^{N_0} (c_{1j} \Phi_j + c_{2j} \Psi_j, \Phi_i), \quad i = 1, 2, \ldots, N_0, \\
\sum_{j=1}^{N_0} a(c_{1j} \Phi_j + c_{2j} \Psi_j, \Psi_i) &= \lambda \sum_{j=1}^{N_0} (c_{1j} \Phi_j + c_{2j} \Psi_j, \Psi_i), \quad i = 1, 2, \ldots, N_0,
\end{align*}
\]
where \( \{c_{1j}, c_{2j}\} \) represent the unknowns. Equivalently,
\[
\tilde{A} \tilde{v} = \tilde{\lambda} \tilde{B} \tilde{v},
\]
where $\tilde{v} = (c_{11}, c_{12}, \ldots, c_{1N_0}, c_{21}, c_{22}, \ldots, c_{2N_0})^T$ and

$$\tilde{A} = \begin{bmatrix} \tilde{A}_{[11]} & \tilde{A}_{[12]} \\ \tilde{A}_{[21]} & \tilde{A}_{[22]} \end{bmatrix}, \quad \tilde{B} = \begin{bmatrix} \tilde{B}_{[11]} & \tilde{B}_{[12]} \\ \tilde{B}_{[21]} & \tilde{B}_{[22]} \end{bmatrix}. $$

A simple calculation shows

$$\tilde{A}_{[11]} = \frac{2}{g} A_{[11]},$$

$$\tilde{A}_{[12]} = \frac{2}{g} \left( \Gamma^{(v)}(S)_{11} A_{[11]} + \Gamma^{(v)}(S)_{12} A_{[12]} \right),$$

$$\tilde{A}_{[21]} = \frac{2}{g} \left( \Gamma^{(v)}(S)_{11} A_{[11]} + \Gamma^{(v)}(S)_{12}^* A_{[21]} \right),$$

$$\tilde{A}_{[22]} = \frac{2}{g} \left\{ \Gamma^{(v)}(S)_{11} \left( \Gamma^{(v)}(S)_{11}^* A_{[11]} + \Gamma^{(v)}(S)_{12}^* A_{[12]} \right) \right. + \\ \left. \Gamma^{(v)}(S)_{12} \left( \Gamma^{(v)}(S)_{11}^* A_{[12]} + \Gamma^{(v)}(S)_{12}^* A_{[22]} \right) \right\}. $$

Let

$$Q_l = \begin{bmatrix} I_{N_0 \times N_0}^{N_0 \times N_0} & 0_{N_0 \times N_0}^{N_0 \times N_0} \\ \Gamma^{(v)}(S)_{11} I_{N_0 \times N_0}^{N_0 \times N_0} & \Gamma^{(v)}(S)_{12} I_{N_0 \times N_0}^{N_0 \times N_0} \end{bmatrix}, \quad Q_r = \begin{bmatrix} I_{N_0 \times N_0}^{N_0 \times N_0} & \Gamma^{(v)}(S)_{11} I_{N_0 \times N_0}^{N_0 \times N_0} \\ 0_{N_0 \times N_0}^{N_0 \times N_0} & \Gamma^{(v)}(S)_{12} I_{N_0 \times N_0}^{N_0 \times N_0} \end{bmatrix},$$

we have

$$Q_l A Q_r = \frac{g}{2} \tilde{A}. $$

Similarly

$$Q_l B Q_r = \frac{g}{2} \tilde{B}. $$

Thus, in the case of $d_v = 2$, we get

$$\lambda = \tilde{\lambda}, \quad v = Q_r \tilde{v},$$

i.e.,

$$u_{1j} = c_{1j} + \Gamma^{(v)}(S)_{11} c_{2j}, \quad u_{2j} = \Gamma^{(v)}(S)_{12} c_{2j}, \quad j = 1, 2, \ldots, N_0. $$

We should point out that the coupled eigenvalue problem appeared in our approach is not an induced complexity. The approach which uses symmetry-adapted bases seems to have an obvious advantage over our approach that the $d_v$ matrix eigenvalue subproblems are decoupled. In fact, the $d_v$ matrix subproblems are the same if following the construction procedure of symmetry-adapted bases in Sect. 3.2. And Theorem 2 tells that the number of symmetry-adapted bases for each $l \in \{1, 2, \ldots, d_v\}$ is $d_v N_0$, which is the size of the matrix problem corresponding to our $d_v$ coupled discretized subproblems. We see that the coupled eigenvalue problem in our approach reflects the essence of irreducible representations of dimensionality larger than one.

Solving subproblems instead of the original eigenvalue problem shall reduce the computational overhead and memory requirement. Each subproblem requires only a smaller number of eigenpairs. And due to the symmetry characteristics, we only need to store and compute part of the degrees of freedom, namely, the degrees of freedom in the irreducible subdomain. Then the solution over the whole domain can be obtained by applying the symmetry characteristic, which does not induce any additional error. Moreover, as indicated in Sect. 2, there
is a possibility to improve the spectral separation, which would accelerate convergence of iterative diagonalization. In the next section, we shall propose a way to analyze the practical decrease in the computational cost.

### 4 Complexity and Performance Analysis

One advantage of solving subproblems (13) instead of the original problem (10) is the reduction in computational cost. By complexity analysis, we estimate the practical speedup in CPU time. In our computation, the algebraic eigenvalue problem is solved by the implicitly restarted Lanczos method (IRLM) in ARPACK package [25]. Actually our analysis can be extended to general Krylov subspace iteration methods.

Total flops of an iterative method are the product of the number of iteration steps and the number of flops per iteration. Most of the flops per IRLM iteration are consumed by three procedures. First is the Schur decomposition of a tridiagonal Hermitian matrix size of \( m \), which consumes about \( 6m^2 \) flops [16]. Second is the \( l \)-step QR iteration with shifts consuming about \( 4lmN \) flops. Third is the \( l \)-step Lanczos factorization, which requires \( l \) matrix-vector multiplication operations. If the shift-invert mode in ARPACK is employed to solve the generalized eigenvalue problem, the matrix-vector multiplication needs to be realized by some iterative linear solver. So the complexity of the third part can be represented as \( O(lN) \). In Table 1 we explain the above notations in complexity analysis.

In total, the complexity per IRLM iteration can be estimated as

\[
 f(l, m, N) = l(4mN + O(N)).
\]  

(21)

In order to clarify the savings in flops per iteration from solving subproblems instead of the original eigenvalue problem, we rewrite (21) as follows

\[
 f(l, m, N) = f_1(l, m, N) + f_2(l, m, N),
\]  

(22)

where \( f_1(l, m, N) = 4lmN \) and \( f_2(l, m, N) = O(lN) \).

In solving the original eigenvalue problem (10), the major flops per IRLM iteration can be counted as (21) or (22). In the decomposition approach, as discussed in Sect. 3.1, we shall solve \( n_c \) decoupled matrix eigenvalue problems and the size of the \( v \)th one is \( d_vN_0 \). In solving the \( v \)th problem (13), \( m \) is reduced to \( m/\theta_1 \), \( N \to d_vN/g \), and \( l \) to \( l/\theta_2 \), where \( g \) is the order of finite group \( G \), \( \theta_1 > 1 \) and \( \theta_2 \approx \theta_1 \) because \( l \) is almost proportional to \( m \). We shall explain in Sect. 5.2 that the number of required eigenpairs for each subproblem is set as the same in the computation, so all the subproblems have an identical \( \theta_1 \). Thus, the majority of total flops per iteration for all \( n_c \) decomposed eigenvalue problems is

---

**Table 1** Notations in complexity analysis

| Notation | Description |
|----------|-------------|
| \( m \)  | The maximum dimension of the Krylov subspace, Twice the number of required eigenpairs plus 5 in our computation |
| \( l \)  | The number of Lanczos factorization steps, s.t. \( m \geq l \) |
| \( N \)  | The number of degrees of freedom, i.e. the size of the matrix, s.t. \( N \gg m \). |
\[
\sum_{\nu=1}^{n_c} f\left(\frac{l}{\theta_2}, \frac{m}{\theta_1}, \frac{d_v N}{g}\right) = \sum_{\nu=1}^{n_c} \left(f_1\left(\frac{l}{\theta_2}, \frac{m}{\theta_1}, \frac{d_v N}{g}\right) + f_2\left(\frac{l}{\theta_2}, \frac{m}{\theta_1}, \frac{d_v N}{g}\right)\right)
= \frac{n_{sub}}{g} \left(\frac{1}{\theta_1} f_1(l, m, N) + \frac{1}{\theta_2} f_2(l, m, N)\right),
\]

where \(n_{sub} = \sum_{\nu=1}^{n_c} d_v\) is the number of subproblems.

Since the complexity in \(f_1\) is different from that in \(f_2\), the speedup in CPU time cannot be directly estimated from (23). Hence we introduce the CPU time ratio \(\omega\) of the matrix-vector multiplications to the whole IRLM process in solving the original eigenvalue problem (10). It is an a posteriori parameter which screens affects of implementation, the runtime environment, as well as the specific linear solver for the shift-invert mode. Besides, testing for \(\omega\) is feasible as the operation of matrix-vector multiplication is usually provided by users.

Applying the symmetry-based decomposition approach instead of solving (10) directly, we can show the speedup in CPU time of one IRLM iteration as follows:

\[
s(\theta_1, \theta_2, \omega) = \frac{1}{\omega} n_{sub} \left(\frac{1}{\theta_1} \frac{1-\omega}{\theta_2} + \frac{1}{\theta_2}\right) = \frac{g\theta_1\theta_2}{n_{sub} \left(1 + (\theta_1 - 1)\omega\right)}.
\]

That is

\[
s(\theta_1, \theta_2, \omega) \approx \frac{g\theta_1^2}{n_{sub} \left(1 + (\theta_1 - 1)\omega\right)}.
\]

In practice, \(\theta_2\) is actually determined by the internal configurations of algebraic eigenvalue solvers. So we prefer to use (24) to predict the CPU time speedup before solving subproblems (13).

In Sect. 6.2, the validation of (24) will be well supported by our numerical experiments. Moreover, this performance analysis implies that the speedup will be amplified when more eigenpairs are required and a consequent decrease in \(\omega\) is very likely. Therefore, the symmetry-based decomposition will be attractive for large-scale eigenvalue problems.

### 5 Practical Issues

In this section, we address some key issues in the implementation of the symmetry-based decomposition approach under grid-based discretizations. We introduce a two-level parallelization for our approach, which leads to a further saving in the CPU time.

#### 5.1 Implementation of Symmetry Characteristics

Symmetry characteristics play a critical role in the decomposition approach, so it is important to preserve and realize symmetry characteristics for discretized eigenfunctions.

For all the degrees of freedom not lying on symmetry elements, the implementation of symmetry characteristics is straightforward with grid-based discretizations. If \(x \in \Omega\) is a degree of freedom lying on the symmetry element corresponding to operation \(R \in G\), the symmetry characteristic

\[
u_l^{(v)}(Rx) = \sum_{m=1}^{d_v} \Gamma_l^{(v)}(R)_{lm} \nu_m^{(v)}(x)
\]
reduces to
\[ u^{(v)}_1(x) = \sum_{m=1}^{d_v} \Gamma^{(v)}_m(R^*) \Gamma^{(v)}_m u^{(v)}_m(x). \]

If \( \det \left( \Gamma^{(v)}(R) - I_{d_v \times d_v} \right) \neq 0 \), then all values \( u^{(v)}_1(x), \ldots, u^{(v)}_{d_v}(x) \) are zeros. Otherwise, we have to find the independent ones out of \( u^{(v)}_1(x), \ldots, u^{(v)}_{d_v}(x) \) and treat them as additional degrees of freedom.

In our computation, we discretize the problem on a tensor-product grid associated with the symmetry group. Currently, for simplicity, we use symmetry groups with symmetry elements on the coordinate planes, and prevent degrees of freedom from lying on the symmetry elements, by imposing an odd number of partition in each direction and using finite elements of odd orders.

5.2 Distribution of Required Eigenpairs Among Subproblems

The required eigenpairs of the original eigenvalue problem (10) are distributed among associated subproblems, and the number of eigenpairs required by each subproblem can be almost reduced by as many times as the number of subproblems. However, we are not able to see in advance the symmetry properties of eigenfunctions corresponding to required eigenvalues. Thus we have to consider some redundant eigenvalues for each subproblem.

We suppose to solve the first \( N_e \) smallest eigenvalues of the original problem. First we set the number of eigenvalues to be computed for each subproblem as \( N_{e,\text{sub}} = \sum_{\nu=1}^{n_{\nu}} d_{\nu} \) plus redundant eigenvalues, where \( n_{\text{sub}} = \sum_{\nu=1}^{n_{\nu}} d_{\nu} \) is the number of subproblems. After solving the subproblems, we gather eigenvalues from all subproblems and sort them in the ascending order. After taking \( N_e \) smallest eigenvalues, we check which subproblems the remaining eigenvalues belong to. If there is no eigenvalue left for some subproblem, the number of computed eigenvalues for this subproblem is probably not enough. Subsequently we restart computing the subproblem with an increased number of required eigenpairs.

5.3 Two-Level Parallel Implementation

We have addressed in Sect. 3 that the \( n_c \) decomposed problems are independent to each other and can be solved simultaneously. Accordingly we have a two-level parallel implementation illustrated by Fig. 1. At the first level, we dispatch the \( n_c \) decomposed problems among groups of processors. At the second level, we distribute the grids among each group of processors. Since eigenfunctions of different subproblems are naturally orthogonal, there is no communication between different groups of processors during solving the eigenvalue problem. Such two-level or multi-level parallelism is likely appreciable for the architecture hierarchy of modern supercomputers. We shall see in Sect. 6.2 that the two-level parallel implementation does reduce the communication cost.

6 Numerical Experiments

In this section, we validate our decomposition approach on a model eigenvalue problem for Abelian and non-Abelian symmetry groups, and show the reduction in computational and communication overhead. Then we apply the approach to electronic structure calculations of symmetric clusters and illustrate the effectiveness of the approach through large-scale
computations. Currently, we use hexahedral finite element discretizations and consider the crystallographic point groups of which symmetry operations keep the hexahedral grids invariant. Our computing platform is the LSSC-III cluster provided by State Key Laboratory of Scientific and Engineering Computing (LSEC), Chinese Academy of Sciences.

6.1 Validation of Implementation

First we validate the implementation of the decomposition approach. Consider a model eigenvalue problem as follows

\[
\begin{align*}
\{-\Delta u &= \lambda u, \quad \text{in } \Omega = (-1, 1)^3, \\
u &= 0, \quad \text{on } \partial \Omega.
\end{align*}
\]  

(25)

The exact eigenvalues are given as

\[\lambda_{k,m,n} = \frac{\pi^2}{4} (k^2 + m^2 + n^2), \quad k, m, n = 1, 2, \ldots.\]

Obviously, the system has all the cubic symmetries. As representatives, we test Abelian subgroup \(D_{2h}\) and non-Abelian subgroups \(D_4\) and \(D_{2d}\). Table 2 gives the irreducible representation matrices of these groups \([8]\), where

\[
\begin{align*}
S_1 &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, &
S_2 &= \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, &
S_3 &= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, &
S_4 &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \\
S_5 &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, &
S_6 &= \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, &
S_7 &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, &
S_8 &= \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.
\end{align*}
\]

According to Theorem 1, we can decompose the original eigenvalue problem (25) as follows:

1. Applying \(D_{2h}\), we have 8 completely decoupled subproblems.
2. Applying \(D_4\) or \(D_{2d}\), we have 6 subproblems and two of them corresponding to representation \(\Gamma(5)\) are coupled eigenvalue problems.

The irreducible subdomain \(\Omega_0\) under the three groups are marked out in Fig. 2. The volume of \(\Omega_0\) is one eighth of \(\Omega\) for all the three groups.
Table 2  Representation matrices of Abelian group $D_{2h}$ and non-Abelian groups $D_4$ and $D_{2d}$

| $D_{2h}$ | $E$ | $C_{2x}$ | $C_{2e}$ | $C_{2f}$ | $I$ | $IC_{2x}$ | $IC_{2e}$ | $IC_{2f}$ |
|---------|-----|---------|---------|---------|----|----------|----------|----------|
| $r^{(1)}$ | 1   | 1       | 1       | 1       | 1  | 1        | 1        | 1        |
| $r^{(2)}$ | 1   | 1       | $-1$   | $-1$   | 1  | 1        | $-1$     | $-1$     |
| $r^{(3)}$ | 1   | $-1$   | 1       | $-1$   | 1  | $-1$    | 1        | $-1$     |
| $r^{(4)}$ | 1   | $-1$   | $-1$   | 1       | 1  | $-1$    | $-1$     | 1        |
| $r^{(5)}$ | 1   | 1       | 1       | 1       | 1  | 1        | 1        | 1        |
| $r^{(6)}$ | 1   | 1       | $-1$   | $-1$   | 1  | $-1$    | $-1$     | 1        |
| $r^{(7)}$ | 1   | $-1$   | $-1$   | 1       | 1  | $-1$    | 1        | $-1$     |
| $r^{(8)}$ | 1   | $-1$   | $-1$   | 1       | 1  | 1        | 1        | $-1$     |

| $D_4$ | $E$ | $C_{2y}$ | $C_{4y}$ | $C_{4y}^{-1}$ | $C_{2x}$ | $C_{2z}$ | $C_{2c}$ | $C_{2d}$ |
|-------|-----|---------|---------|--------------|---------|---------|---------|---------|
| $r^{(1)}$ | 1   | 1       | 1       | 1            | 1       | 1       | 1       | 1       |
| $r^{(2)}$ | 1   | 1       | $-1$   | $-1$         | 1       | 1       | $-1$   | $-1$   |
| $r^{(3)}$ | 1   | 1       | 1       | 1            | $-1$   | $-1$   | 1       | $-1$   |
| $r^{(4)}$ | 1   | 1       | $-1$   | $-1$         | $-1$   | 1       | $-1$   | 1       |
| $r^{(5)}$ | $S_1$ | $S_2$ | $S_3$ | $S_4$ | $S_5$ | $S_6$ | $S_7$ | $S_8$ |

| $D_{2d}$ | $E$ | $C_{2y}$ | $IC_{4y}$ | $IC_{4y}^{-1}$ | $IC_{2x}$ | $IC_{2z}$ | $C_{2c}$ | $C_{2d}$ |
|---------|-----|---------|----------|--------------|---------|---------|---------|---------|
| $r^{(1)}$ | 1   | 1       | 1        | 1            | 1       | 1       | 1       | 1       |
| $r^{(2)}$ | 1   | 1       | $-1$   | $-1$         | 1       | 1       | $-1$   | $-1$   |
| $r^{(3)}$ | 1   | 1       | 1       | 1            | $-1$   | $-1$   | 1       | $-1$   |
| $r^{(4)}$ | 1   | 1       | $-1$   | $-1$         | $-1$   | 1       | $-1$   | 1       |
| $r^{(5)}$ | $S_1$ | $S_2$ | $-S_3$ | $-S_4$ | $-S_5$ | $-S_6$ | $S_7$ | $S_8$ |

All the three groups have 8 symmetry operations, i.e., order $g = 8$. Abelian group $D_{2h}$ has $n_c = 8$ one-dimensional irreducible representations, and both the two non-Abelian groups have $n_c = 5$ irreducible representations, one of which is two-dimensional. A description about the notation of symmetry operations in the table is given in Appendix 1

![Fig. 2 Illustration of irreducible subdomain $\Omega_0$.](a) For $D_{2h}$ it is a small cube; (b) For $D_4$, a triangular prism; (c) For $D_{2d}$ also a triangular prism, with a different shape)

We employ trilinear finite elements to solve these eigenvalue subproblems, and see from the convergence rate of eigenvalues that the implementation is correct. Taking non-Abelian
Fig. 3 Errors in the eigenvalue approximations from solving 6 subproblems associated with non-Abelian group $D_4$ using trilinear finite elements. Errors in the first three different eigenvalues $\frac{3}{4}\pi^2$, $\frac{3}{2}\pi^2$ and $\frac{9}{4}\pi^2$ are labeled as $e_1$, $e_2$ and $e_5$, respectively. The $h^2$-convergence rate can be observed.

Table 3 The $\nu$-$l$ symmetries of the first 10 computed eigenfunctions from solving subproblems

|     | $u_1$ | $u_2$ | $u_3$ | $u_4$ | $u_5$ | $u_6$ | $u_7$ | $u_8$ | $u_9$ | $u_{10}$ |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|----------|
| $D_{2h}$ | $\nu$ | 1     | 8     | 7     | 6     | 4     | 2     | 3     | 1     | 1        |
|       | $l$   | 1     | 1     | 1     | 1     | 1     | 1     | 1     | 1     | 1        |
| $D_4$ | $\nu$ | 1     | 3     | 5     | 5     | 4     | 5     | 5     | 2     | 1        |
|       | $l$   | 1     | 1     | 1     | 2     | 1     | 1     | 2     | 1     | 1        |
| $D_{2d}$ | $\nu$ | 1     | 2     | 5     | 5     | 4     | 5     | 5     | 1     | 2        |
|       | $l$   | 1     | 1     | 1     | 2     | 1     | 1     | 2     | 1     | 1        |

The $\nu$-$l$ values indicate which subproblem each eigenfunction belongs to, where $\nu \in \{1, 2, \ldots, n_c\}$ and $l \in \{1, 2, \ldots, d_\nu\}$. In the case of $D_{2h}$, all the $l$ values are 1 because it is an Abelian group and all irreducible representations are one-dimensional, i.e., $d_\nu = 1$ for all $\nu = 1, 2, \ldots, 8$.

Taking Abelian group $D_{2h}$ as an example, we compare the computational cost of solving the original eigenvalue problem (25) with that of solving 8 subproblems. We compute the first 110 eigenvalues of the original eigenvalue problem. And it is sufficient to solve the first 22
Table 4  Statistics of solving the original problem (25) and 8 subproblems using trilinear finite elements

In Column 1, subproblems are labeled by different $\nu$ values. Columns 2 and 3 list the number of iteration steps and matrix-vector multiplications. Columns 4 and 5 give the CPU time spent on matrix-vector multiplications and the whole procedure of IRLM.

| Problem | #Iter. | #OP*$x$ | time_mv (sec.) | time_total (s) |
|---------|--------|---------|----------------|----------------|
| (25)    | 33     | 2,304   | 318.48         | 1,892.32       |

\[
\begin{align*}
\nu = 1 & \quad 32 \quad 555 \quad 10.21 \quad 17.95 \\
\nu = 2 & \quad 26 \quad 488 \quad 8.85 \quad 15.53 \\
\nu = 3 & \quad 25 \quad 474 \quad 8.50 \quad 14.88 \\
\nu = 4 & \quad 24 \quad 461 \quad 8.31 \quad 14.59 \\
\nu = 5 & \quad 28 \quad 490 \quad 8.79 \quad 15.95 \\
\nu = 6 & \quad 27 \quad 503 \quad 8.72 \quad 15.78 \\
\nu = 7 & \quad 23 \quad 452 \quad 7.97 \quad 14.17 \\
\nu = 8 & \quad 25 \quad 478 \quad 8.36 \quad 14.92
\end{align*}
\]

Table 5  Statistics of solving (25) and 8 subproblems using tricubic finite elements

| Problem | #Iter. | #OP*$x$ | Time_mv (s) | Time_total (s) |
|---------|--------|---------|-------------|----------------|
| (25)    | 70     | 4,834   | 2,593.81    | 5,554.60       |

\[
\begin{align*}
\nu = 1 & \quad 83 \quad 1,384 \quad 102.66 \quad 120.21 \\
\nu = 2 & \quad 59 \quad 1,076 \quad 78.60 \quad 91.47 \\
\nu = 3 & \quad 54 \quad 1,012 \quad 74.36 \quad 86.37 \\
\nu = 4 & \quad 58 \quad 1,062 \quad 77.55 \quad 90.30 \\
\nu = 5 & \quad 62 \quad 1,068 \quad 78.41 \quad 91.78 \\
\nu = 6 & \quad 52 \quad 992 \quad 73.28 \quad 84.96 \\
\nu = 7 & \quad 52 \quad 992 \quad 72.83 \quad 84.52 \\
\nu = 8 & \quad 52 \quad 991 \quad 72.66 \quad 84.30
\end{align*}
\]

eigenvalues of each subproblem. In order to illustrate and analyze the saving in computational cost, we launch the tests on a single CPU core.

In Table 4, we present statistics from trilinear finite element discretizations. We see that the average CPU time of a single iteration during solving the original problem (25) is 57.34 seconds while that of solving 8 subproblems is 4.73 seconds. In Table 5, we present statistics from tricubic finite element discretizations. We observe that the average CPU time of a single iteration during solving the original problem (25) is 79.35 seconds while that of solving 8 subproblems is 12.52 seconds.

We note that the speedup in average CPU time of a single iteration is 12.12 with trilinear finite elements while it is decreased to 6.34 with tricubic finite elements. This numerical phenomenon can be explained by performance analysis (24). In our computation, the maximum dimension of Krylov subspace is twice the number of required eigenpairs plus 5, which is recommended by ARPACK’s tutorial examples. So we have $\theta_1 = 4.59$. We obtain from the statistics of solving the original problem that the CPU time percentage $\omega$ of matrix-vector multiplications is 0.17 with trilinear finite elements and grows to 0.47 with tricubic finite elements. Correspondingly, using (24), we can predict that the CPU time speedup for trilinear and tricubic finite elements would be 13.08 and 7.84, respectively.

---

4 We count the average CPU time of a single iteration for each subproblem and then accumulate them. Taking Table 4 for example, we have that $4.73 = 17.95/32 + 15.53/26 + 14.88/25 + 14.59/24 + 15.95/28 + 15.78/27 + 14.17/23 + 14.92/25$. 

Springer
Table 6 Comparison of communication between solving (25) and 8 subproblems

| N_p | N_p in comm. | Bytes in comm. | CPU time in comm. (s) |
|-----|--------------|----------------|----------------------|
|     | Use symm.    | Use symm.      |                      |
|     | Not use      | Not use        |                      |
| 8   | 0.00         | 1.75           | 0                    |
|     |              | 134,560        | 0.00                 |
|     |              |                | 11.95                |
| 16  | 1.00         | 1.88           | 19,608               |
|     |              | 145,451        | 0.24                 |
|     |              |                | 14.30                |

Column 1 gives the number of processors. In the other columns, “use symm” represents solving subproblems and “not use” means solving the original eigenvalue problem. Columns 2 and 3 give the average number of processors each processor communicates with. Columns 4 and 5 list the average number of bytes sent by each processor. And the last two columns report the CPU time spent on communication during matrix-vector multiplications.

We see from (22) that the computational cost of QR-iteration grows faster than that of matrix-vector multiplication when the number of required eigenpairs increases. Thus we can expect that the decomposition approach would be more attractive for large-scale eigenvalue problems.

Besides the reduction in computational cost, solving decoupled problems will also save communication among parallel processors. As mentioned in Sect. 5.3, our implementation of the decomposition approach is parallelized in two levels. No communication occurs between any two groups of processors during solving the eigenvalue problem. This leads to a saving in communication. For illustration, we still take eigenvalue problem (25) and decompose it into 8 decoupled subproblems according to group $D_{2h}$. The comparison of communication between solving the original problem and the subproblems is given in Table 6.

6.3 Applications to Electronic Structure Calculations

Density functional theory (DFT) provides a powerful tool to study physical, mechanical and chemical properties of many-electron systems [21,26]. In the context of DFT, the central problem is to solve the Kohn–Sham equation which is a nonlinear eigenvalue problem [21,22]. The dominant part of computation is the repeated solving of the linearized eigenvalue problem along with the self-consistent field (SCF) iteration [26]. The number of required eigenstates grows in proportion to that of valence electrons in the system. Thus the Kohn–Sham equation solver will probably make the performance bottleneck for large-scale DFT calculations. To reduce the computational cost, in this section, we apply the decomposition approach to solving the Kohn–Sham equations of symmetric cluster systems. We shall show that our decomposition approach and the two-level parallelization can reduce the CPU time remarkably and would be attractive for large-scale eigenvalue problems.

Compared with classical methods, we see that grid-based discretizations are easy to handle cluster or surface systems, and the locality in them is favorable for parallel computing [4,35]. In the last two decades, grid-based discretizations have been successfully applied to electronic structure calculations, see, e.g., [1,11,12,18,31,33,37,38,41]) for finite element methods, [7,19,23,30] for finite difference, and [10,15] for others like the finite volume method and wavelet approach. However, we note that there is few work on the exploitation of symmetry with grid-based discretizations.

Recall that the Kohn–Sham equation is a nonlinear eigenvalue problem as follows

$$\left(-\frac{1}{2}\Delta + V_{\text{eff}}[\rho]\right)\psi_n = \epsilon_n \psi_n \quad \text{in} \, \mathbb{R}^3,$$

(26)
Table 7  Representation matrices of Abelian group $D_2$

| $D_2$ | $E$ | $C_{2x}$ | $C_{2y}$ | $C_{2z}$ |
|-------|-----|---------|---------|---------|
| $\Gamma^{(1)}$ | 1   | 1       | 1       | 1       |
| $\Gamma^{(2)}$ | 1   | 1       | -1      | -1      |
| $\Gamma^{(3)}$ | 1   | -1      | 1       | -1      |
| $\Gamma^{(4)}$ | 1   | -1      | -1      | 1       |

where $\rho(\mathbf{r}) = \sum_{n=1}^{N_e} f_n |\Psi_n(\mathbf{r})|^2$ is the charge density contributed by $N_e$ eigenfunctions $\{\Psi_n\}$ with occupancy numbers $\{f_n\}$, and $V^{\text{eff}}[\rho]$ the so-called effective potential which is a nonlinear functional of $\rho$. On the assumption of no external fields, $V^{\text{eff}}[\rho]$ can be written into

$$V^{\text{eff}} = V^{\text{ne}} + V^H + V^{xc},$$

where $V^{\text{ne}}$ is the Coulomb potential between the nuclei and the electrons, $V^H$ the Hartree potential, and $V^{xc}$ the exchange-correlation potential [26]. Since the ground state density of a cluster system decays exponentially [2,14,32], we choose the computational domain as an appropriate cube and impose zero boundary condition.

We compute a series of symmetric carbon clusters and aluminum face-centered cubic (FCC) clusters with tricubic finite elements. Figure 4 illustrates the configuration of these two classes of systems. Our calculations are based on code real space parallel adaptive calculation of electronic structure (RealSPACES) of the LSEC of Chinese Academy of Sciences. We use group $D_2$ for the carbon clusters to decompose (26) into 4 decoupled subproblems, and $D_{2h}$ for aluminum clusters to get 8 decoupled subproblems. Table 7 gives the representation matrices of $D_2$ [8].

Figure 5 shows the charge density of two representative systems. In Table 8, we compare between solving the original Kohn–Sham equation and the decomposed subproblems. It can be seen that our decomposition approach with the two-level parallelization leads to a distinguished saving in the CPU time. The increasing speedup with the scale of system indicates that our approach would be attractive for large-scale symmetric systems. Moreover,

---

5 The configuration is visualized by PyMOL.

6 The charge density is visualized by JADLIB [40] and JAVIS [28] developed by HPCC, Institute of Applied Physics and Computational Mathematics.
Fig. 5 Sectional drawing of charge density of carbon cluster C\textsubscript{885}H\textsubscript{420} on the (0, 0, 1) plane (left) and aluminum FCC cluster Al\textsubscript{1099} on the (1, 1, 1) plane (right).

Table 8 Comparison between solving the original Kohn–Sham equation and subproblems with tricubic finite elements

| System     | \(N_e\) | \(N\)      | \(N_0\) | \(N_p\) | Diag. CPU time | Speedup |
|------------|---------|------------|---------|---------|----------------|---------|
| C\textsubscript{123}H\textsubscript{100} | 300     | 681,472    | 170,368 | 16      | 29 m           | 4 m     | 7.3      |
| C\textsubscript{275}H\textsubscript{172} | 640     | 830,584    | 207,646 | 32      | 1 h 3 m        | 6 m     | 10.5     |
| C\textsubscript{525}H\textsubscript{276} | 1,200   | 1,404,928  | 351,232 | 64      | 2 h 56 m       | 14 m    | 12.6     |
| C\textsubscript{885}H\textsubscript{420} | 2,000   | 2,197,000  | 549,250 | 128     | 6 h 30 m       | 27 m    | 14.4     |
| Al\textsubscript{172}     | 280     | 681,472    | 85,184  | 16      | 44 m           | 3 m     | 14.7     |
| Al\textsubscript{365}     | 600     | 1,191,016  | 148,877 | 32      | 2 h 24 m       | 6 m     | 24.0     |
| Al\textsubscript{666}     | 1,100   | 1,906,624  | 238,328 | 64      | 5 h 59 m       | 11 m    | 32.6     |
| Al\textsubscript{1,099}   | 1,700   | 2,863,288  | 357,911 | 128     | 11 h 11 m      | 15 m    | 44.7     |

Column 2 gives the number of required eigenstates. The number of degrees of freedom given in Columns 3 and 4 is required by the convergence of ground state energy [11]. Columns 6 and 7 list the average CPU time in diagonalization at each SCF iteration step, which is the dominant part of time. The last column is the speedup of the decomposition approach.

the discretization scale in Table 8 illustrates that our approach is friendly to large-scale grid-based discretizations.

Here we have only demonstrated the effectiveness of the decomposition approach and the two-level parallelization from solving some testing systems. We shall report elsewhere the implementation details on the group theoretic finite element Kohn–Sham solver, and the application of the approach to large-scale systems with defects and structural relaxation, etc.

7 Concluding Remarks

We have proposed a decomposition approach to differential eigenvalue problems with Abelian or non-Abelian spatial symmetries, which decompose the differential eigenvalue problem into eigenvalue subproblems characterized by distinct symmetry characteristics. Our approach could be seamlessly incorporated with grid-based discretizations, such as finite difference,
finite element or finite volume methods. The approach can reduce the computational cost remarkably, since each subproblem requires only a smaller number of eigenpairs, and we only need to store and compute part of the degrees of freedom due to the symmetry characteristics.

Different from the classical treatment of symmetry in quantum chemistry, our approach does not explicitly construct symmetry-adapted bases. However, we have provided a construction procedure for the symmetry-adapted bases, from which we have obtained the exact relation between approximate eigenpairs from the two approaches.

We have introduced a two-level parallelization for our approach and implemented it with finite elements for illustration. In particular, we have applied our approach to electronic structure calculations of symmetric clusters, and demonstrated its effectiveness through solving thousands of eigenstates with millions of degrees of freedom. By complexity analysis and numerical examples, we have shown that our approach would be attractive for large-scale eigenvalue problems.

If solving the Kohn–Sham equations of periodic crystals, we should consider plane wave expansion which could be regarded as grid-based discretization in reciprocal space. In Appendix 4, we show that the invariance under some coordinate transformation can be kept by Fourier transformation. So the decomposition approach would be applicable to plane waves, too. We would like to emphasize that, although some plane-wave codes have utilized some symmetry, the symmetry is only used to reduce the number of $k$-points or to symmetrize the charge density. For each given $k$-point, they do not decompose the Kohn–Sham equation according to symmetry characteristics of eigenstates, and thus still solve the original eigenvalue problem.

Currently, we only consider spatial symmetry. It is possible to use other symmetries to reduce the computational cost, too. For instance, the angular momentum, spin and parity symmetries of atoms have been exploited during solving the Schrödinger equation in [13,27]; the total particle number and the total spin $z$-component, except for rotational and translational symmetries, have been taken into account to block-diagonalize the local (impurity) Hamiltonian in the computation of dynamical mean-field theory for strongly correlated systems [17,20]. It is our future work to exploit these underlying or internal symmetries.

Acknowledgments The authors would like to thank Prof. Xiaoying Dai, Prof. Xingao Gong, Prof. Lihua Shen, Dr. Zhang Yang, and Mr. Jinwei Zhu for their stimulating discussions on electronic structure calculations. The second author is grateful to Prof. Zeyao Mo for his encouragement. The authors would also like to thank the referee for his/her constructive comments and suggestions that improved the presentation of this paper.

Appendix 1: Basic Concept of Group Theory

In this appendix, we include some basic concepts of group theory for a more self-contained exposition. They could be found in standard textbooks like [8,9,34].

A group $G$ is a set of elements $\{R\}$ with a well-defined multiplication operation which satisfy the following requirements:

1. The set is closed under the multiplication.
2. The associative law holds.
3. There exists a unit element $E$ such that $ER = RE = R$ for any $R \in G$.
4. There is an inverse $R^{-1}$ in $G$ to each element $R$ such that $RR^{-1} = R^{-1}R = E$.

If the commutative law of multiplication also holds, $G$ is called an Abelian group. Group $G$ is called a finite group if it contains a finite number of elements. And this number, denoted...
by \( g \), is said to be the order of the group. The rearrangement theorem tells that the elements of \( G \) are only rearranged by multiplying each by any \( R \in G \), i.e., \( RG = G \) for any \( R \in G \).

An element \( R_1 \in G \) is called to be conjugate to \( R_2 \) if \( R_2 = SR_1S^{-1} \), where \( S \) is some element in the group. All the mutually conjugate elements form a class of elements. It can be proved that group \( G \) can be divided into distinct classes. Denote the number of classes as \( n_c \). In an Abelian group, any two elements are commutative, so each element forms a class by itself, and \( n_c \) equals the order of the group.

Groups \( G = \{ R \} \) and \( G' = \{ R' \} \) are called to be homomorphic, if there exists a correspondence between the elements of \( G \) and \( G' \) as \( R \leftrightarrow R'_1, R'_2, \ldots \), which means that if \( RS = T \) then the product of any \( R'_i \) with any \( S'_j \) will belong to the set \( \{ T'_1, T'_2, \ldots \} \). This is a many-to-one correspondence in general. If the correspondence specializes to be one-to-one, the two groups are called to be isomorphic.

A matrix representation of group \( G \) means a group of matrices which is homomorphic to \( G \). Two representations are said to be equivalent if they are associated by a similarity transformation. If a representation can not be equivalent to representations of lower dimensionality, it is called irreducible. Any matrix representation with nonzero determinants is equivalent to a unitary representation, i.e., a representation by unitary matrices.

The number of all the inequivalent, irreducible, unitary representations is equal to \( n_c \), which is the number of classes in \( G \). The Celebrated Theorem tells that

\[
\sum_{\nu=1}^{n_c} d_{\nu}^2 = g,
\]

where \( d_{\nu} \) denotes the dimensionality of the \( \nu \)th representation. Since the number of classes of an Abelian group equals the number of elements, an Abelian group of order \( g \) has \( g \) one-dimensional irreducible representations.

The groups used in this paper are all crystallographic point groups. Groups \( D_2, \ D_{2h}, \ D_{2d} \) and \( D_4 \) are four dihedral groups; the first two groups are Abelian and the other two are non-Abelian. In Tables 2 and 7, \( C_{nj} \) denotes a rotation about axis \( Oj \) by \( 2\pi/n \) in the right-hand screw sense and \( I \) is the inversion operation [8]. The \( Oj \) axes are illustrated in Fig. 6. We refer to textbooks like [8,9,34] for more details about crystallographic point groups.
Appendix 2: Proof of Proposition 2

Proof (a) Since \( \{ P_R \} \) are unitary operators, we have

\[
\mathcal{P}_{ml}^{(v)*} = \frac{d_v}{g} \sum_{R \in G} \Gamma^{(v)}(R)_{ml} P_R = \frac{d_v}{g} \sum_{S \in G} \Gamma^{(v)}(S^{-1})_{ml} P_S,
\]

which together with the fact that \( \Gamma^{(v)} \) is a unitary representation derives

\[
\mathcal{P}_{ml}^{(v)*} = \frac{d_v}{g} \sum_{S \in G} \Gamma^{(v)}(S)_{lm} P_S = \mathcal{P}_{lm}^{(v)}.
\]

(b) It follows from the definition that

\[
\mathcal{P}_{ml}^{(v)} \mathcal{P}_{m'l'}^{(v')} = \left( \frac{d_v}{g} \sum_{R \in G} \Gamma^{(v)}(R)_{ml} P_R \right) \left( \frac{d_{v'}}{g} \sum_{S \in G} \Gamma^{(v')}(S)_{m'l'} P_S \right)
\]

\[
= \frac{d_v d_{v'}}{g^2} \sum_{R \in G} \Gamma^{(v)}(R)_{ml} \left( \sum_{S \in G} \Gamma^{(v')}(S)_{m'l'} P_S \right).
\]

Note that the rearrangement theorem implies that, when \( S \) runs over all the group elements, \( S' = RS \) for any \( R \) also runs over all the elements. Hence we get

\[
\mathcal{P}_{ml}^{(v)} \mathcal{P}_{m'l'}^{(v')} = \frac{d_v d_{v'}}{g^2} \sum_{S \in G} \left( \sum_{R \in G} \Gamma^{(v)}(R)_{ml} \Gamma^{(v')}(R^{-1}S')_{m'l'} P_S \right).
\]

We may calculate as follows

\[
\sum_{R \in G} \Gamma^{(v)}(R)_{ml} \Gamma^{(v)}(R^{-1}S')_{m'l'} = \sum_{R \in G} \Gamma^{(v)}(R)_{ml} \left( \sum_{n=1}^{d_v} \Gamma^{(v')}(R^{-1}S')_{m'n} \Gamma^{(v)}(S')_{nl'} \right)
\]

\[
= \sum_{R \in G} \Gamma^{(v)}(R)_{ml} \left( \sum_{n=1}^{d_{v'}} \Gamma^{(v')}(R)_{nm'} \Gamma^{(v)}(S')_{nl'} \right)
\]

\[
= \sum_{n=1}^{d_v} \Gamma^{(v')}(S')_{nl'} \left( \sum_{R \in G} \Gamma^{(v)}(R)_{ml} \Gamma^{(v')}(R)_{nm'} \right),
\]

which together with the great orthogonality theorem yields

\[
\sum_{R \in G} \Gamma^{(v)}(R)_{ml} \Gamma^{(v')}(R^{-1}S')_{m'l'} = \delta_{vv'}\delta_{lm'} \frac{g}{d_{v'}} \Gamma^{(v)}(S')_{m'l'}.
\]

Thus we arrive at

\[
\mathcal{P}_{ml}^{(v)} \mathcal{P}_{m'l'}^{(v')} = \delta_{vv'}\delta_{lm'} \frac{d_v}{g} \sum_{S' \in G} \Gamma^{(v)}(S')_{ml'} P_{S'} = \delta_{vv'}\delta_{lm'} \mathcal{P}_{ml}^{(v')}.
\]

\[\square\]
Moreover, the first subproblem does not have this eigenvalue, which shows that nondegenerate for subproblems. This implies a relation between symmetry and degeneracy. In other words, a doubly-degenerate eigenvalue of the original problem becomes a relation in Corollary 2. Namely, we consider the decomposition of the following eigenvalue equation in (23), for the 4 subproblems are

\[ \sum_{i} E_{i} R_{i} = E \]

Note that \( G = \{ E, \sigma_{x}, \sigma_{y}, I \} \) is a symmetry group associated with (27), where \( E \) represents the identity operation, \( \sigma_{x} \) a reflection about \( x \)-axis, \( \sigma_{y} \) a reflection about \( y \)-axis, and \( I \) the inversion operation. We see that \( G \) is an Abelian group of order 4, and has 4 one-dimensional irreducible representations as shown in Table 9.

According to Theorem 1 and Corollary 2, eigenvalue problem (27) can be decomposed into 4 subproblems (due to \( \sum_{i} d_{i} = 4 \)). And the symmetry characteristic conditions, the third equation in (13), for the 4 subproblems are

| \( G \) | \( R_1 = E \) | \( R_2 = \sigma_x \) | \( R_3 = \sigma_y \) | \( R_4 = I \) |
|---|---|---|---|---|
| \( \Gamma^{(1)} \) | 1 | 1 | 1 | 1 |
| \( \Gamma^{(2)} \) | 1 | 1 | -1 | -1 |
| \( \Gamma^{(3)} \) | 1 | -1 | -1 | 1 |
| \( \Gamma^{(4)} \) | 1 | -1 | 1 | -1 |

where \( x \in \Omega \) is an arbitrary point and subscripts of \( u^{(v)} \) are omitted.

In Fig. 7, we illustrate four eigenfunctions of (27) belonging to different subproblems. We see that \( u_2 \) and \( u_3 \) are degenerate eigenfunctions corresponding to \( \lambda = \frac{5}{4} \pi^2 \) with double degeneracy. In other words, a doubly-degenerate eigenvalue of the original problem becomes nondegenerate for subproblems. This implies a relation between symmetry and degeneracy [24,29,36]. Moreover, the first subproblem does not have this eigenvalue, which shows that the decomposition approach has improved the spectral separation.

Appendix 4: Spatial Symmetry in Reciprocal Space

Plane wave method is widely used for solving the Kohn–Sham equations of crystals. Actually, plane waves may be regarded as grid-based discretizations in reciprocal space. We will show that the symmetry relation in real space is kept in reciprocal space. The solution domain \( \Omega \) of crystals can be spanned by three lattice vectors in real space. We denote them as \( \mathbf{a}_i (i = 1, 2, 3) \). If function \( f \) is invariant with integer multiple translations of the lattice vectors, we then present the function in reciprocal space as like:

\[ \hat{f}(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}} f(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} \]
Fig. 7 Four eigenfunctions of problem (27): $u_1$ keeps invariant under $\{E, \sigma_x, \sigma_y, I\}$ and satisfies Eq. (28), and $u_2, u_3$ and $u_4$ satisfy (29), (30) and (31), respectively.

where $\mathbf{q}$ is any vector in reciprocal space satisfying $\mathbf{q} \cdot \mathbf{a}_i = \frac{2\pi n}{N_i}$ with $n$ an integer, $N_i$ the number of degrees of freedom along direction $\mathbf{a}_i$ ($i = 1, 2, 3$), and $N = N_1N_2N_3$ the total number of degrees of freedom. Assume that $f$ is kept invariant under coordinate transformation $R$ in $\Omega$. We obtain from

$$\hat{f}(R\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}} f(\mathbf{r}) e^{-i(R\mathbf{q}) \cdot \mathbf{r}}$$

and the coordinate transformation $R$ can be represented as an orthogonal matrix that

$$\hat{f}(R\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}} f(\mathbf{r}) e^{-i\mathbf{q} \cdot (R^{-1}\mathbf{r})}.$$  

Since

$$f(R^{-1}\mathbf{r}) = f(\mathbf{r}) \quad \forall \mathbf{r} \in \Omega,$$

we have

$$\hat{f}(R\mathbf{q}) = \frac{1}{N} \sum_{R^{-1}\mathbf{r}} f(R^{-1}\mathbf{r}) e^{-i\mathbf{q} \cdot (R^{-1}\mathbf{r})} = \hat{f}(\mathbf{q}).$$

Hence the decomposition approach is probably applicable to plane waves.

References

1. Ackermann, J., Erdmann, B., Roitzsch, R.: A self-adaptive multilevel finite element method for the stationary Schrödinger equation in three space dimensions. J. Chem. Phys. 101, 7643–7650 (1994)
2. Agmon, S.: Lectures on the Exponential Decay of Solutions of Second-Order Elliptic Operators. Princeton University Press, Princeton (1981)
3. Banjai, L.: Eigenfrequencies of fractal drums. J. Comput. Appl. Math. 198, 1–18 (2007)
4. Beck, T.L.: Real-space mesh techniques in density-functional theory. Rev. Mod. Phys. 72, 1041–1080 (2000)
5. Bossavit, A.: Symmetry, groups, and boundary value problems. A progressive introduction to noncommu-
tative harmonic analysis of partial differential equations in domains with geometrical symmetry. Comput.
Methods Appl. Mech. Eng. 56, 167–215 (1986)
6. Bossavit, A.: Boundary value problems with symmetry, and their approximation by finite elements. SIAM
J. Appl. Math. 53, 1352–80 (1993)
7. Chelikowsky, J.R., Troullier, N., Saad, Y.: Finite-difference-pseudopotential method: electronic structure
calculations without a basis. Phys. Rev. Lett. 72, 1240–1243 (1994)
8. Cornwell, J.F.: Group Theory in Physics: An Introduction. Academic Press, California (1997)
9. Cotton, F.A.: Chemical Applications of Group Theory, 3rd edn. Wiley-Interscience, New York (1990)
10. Dai, X., Gong, X., Yang, Z., Zhang, D., Zhou, A.: Finite volume discretizations for eigenvalue problems
with applications to electronic structure calculations. Multiscale Model. Simul. 9, 208–240 (2011)
11. Fang, J., Gao, X., Zhou, A.: A Kohn–Sham equation solver based on hexahedral finite elements. J. Comput.
Phys. 231, 3166–3180 (2012)
12. Fattebert, J.-L., Hornung, R.D., Wissink, A.M.: Finite element approach for density functional theory
calculations on locally-refined meshes. J. Comput. Phys. 223, 759–773 (2007)
13. Friesecke, G., Goddard, B.D.: Asymptotics-based CI models for atoms: properties, exact solution of a
minimal model for Li to Ne, and application to atomic spectra. Multiscale Model. Simul. 7, 1876–1897
(2009)
14. Gârding, L.: On the essential spectrum of Schrödinger operators. J. Funct. Anal. 52, 1–10 (1983)
15. Genovese, L., Neelov, A., Goedecker, S., Deutsch, T., Ghasemi, S.A., Willand, A., Caliste, D., Zilberberg,
O., Rayson, M., Bergman, A., Schneider, R.: Daubechies wavelets as a basis set for density functional
pseudopotential calculations. J. Chem. Phys. 129, 014109 (2008)
16. Golub, G.H., van Loan, C.F.: Matrix Computations. Johns Hopkins University Press, Baltimore (1996)
17. Gull, E., Millis, A.J., Lichtenstein, A.I., Rubtsov, A.N., Troyer, M., Werner, P.: Continuous-time Monte
Carlo methods for quantum impurity models. Rev. Mod. Phys. 83, 349–404 (2011)
18. Gong, X., Shen, L., Zhang, D., Zhou, A.: Finite element approximations for Schrödinger equations with
applications to electronic structure computations. J. Comput. Math. 23, 310–327 (2008)
19. Hasegawa, Y., Iwata, J.-I., Tsuji, M., Takahashi, D., Oshiyama, A., Minami, K., Boku, T., Shoji, F., Uno,
A., Kurokawa, M., Inoue, H., Miyoshi, L., Yokokawa M.: First-principles calculations of electron states
of a silicon nanowire with 100,000 atoms on the K computer. In: Proceedings of 2011 International
Conference for High Performance Computing, Networking, Storage and Analysis (SC2011), pp. 1–11
(2011)
20. Haule, K.: Quantum Monte Carlo impurity solver for cluster dynamical mean-field theory and electronic
calculations with adjustable cluster base. Phys. Rev. B 75, 155113 (2007)
21. Hohenberg, P., Kohn, W.: Inhomogeneous electron gas. Phys. Rev. B 136(3B), B864–B871 (1964)
22. Kohn, W., Sham, L.J.: Self-consistent equations including exchange and correlation effects. Phys. Rev.
140(4A), A1133–A1136 (1965)
23. Kronik, L., Makmal, A., Tiago, M.L., Alemany, M.M.G., Jain, M., Huang, X., Saad, Y., Chelikowsky, J.R.:
Parsec—the pseudopotential algorithm for real-space electronic structure calculations: recent advances
and novel applications to nano-structures. Phys. Stat. Sol. B. 243, 1063–1079 (2006)
24. Kuttler, J.R., Sigillito, V.G.: Eigenvalues of the Laplacian in two dimensions. SIAM Rev. 26, 163–193
(1984)
25. Lehoucq, R.B., Sorensen, D.C., Yang, C.: ARPACK Users’ Guide: Solution of Large-scale Eigenvalue
Problems with Implicitly Restarted Arnoldi Methods. SIAM, Philadelphia (1998)
26. Martin, R.M.: Electronic Structure: Basic Theory and Practical Methods. Cambridge University Press,
Cambridge (2004)
27. Mendl, C.B., Friesecke, G.: Efficient algorithm for asymptotics-based configuration-interaction methods
and electronic structure of transition metal atoms. J. Chem. Phys. 133, 184101 (2010)
28. Mo, Z., Zhang, A., (eds.): User’s guide for JASMIN Technical Report No. T09-JMJL-01. http://www.
iapcm.ac.cn/jasmin (2009)
29. Neuberger, J.M., Sieben, N., Swift, J.W.: Computing eigenfunctions on the Koch Snowflake: a new grid
and symmetry. J. Comput. Appl. Math. 191, 126–142 (2006)
30. Ono, T., Hirose, K.: Real-space electronic-structure calculations with a time-saving double-grid technique.
Phys. Rev. B. 72, 085115 (2005)
31. Pask, J.E., Sterne, P.A.: Finite element methods in ab initio electronic structure calculations. Model.
Simul. Mater. Sci. Eng. 13, 71–96 (2005)
32. Simon, B.: Schrödinger operators in the twentieth century. J. Math. Phys. 41, 3523–3555 (2000)
33. Suryanarayana, P., Gavini, V., Blesgen, T.: Non-periodic finite-element formulation of Kohn–Sham density functional theory. J. Mech. Phys. Solids 58, 256–280 (2010)
34. Tinkham, M.: Group Theory and Quantum Mechanics. McGraw-Hill, New York (1964)
35. Torsti, T., Eirola, T., Enkovaara, J., Hakala, T., Havu, P., Havu, V., Höynälänmaa, T., Ignatius, J., Lyly, M., Makkonen, I., Rantala, T.T., Ruokolainen, J., Ruotsalainen, K., Räisänen, E., Saarikoski, H., Puska, M.J.: Three real-space discretization techniques in electronic structure calculations. Phys. Stat. Sol. B243, 1016–1053 (2006)
36. Trefethen, L.N., Betcke, T., Computed eigenmodes of planar regions. In: Recent advances in differential equations and mathematical physics, volume 412 of Contemp. Math., pp. 297–314. Providence, RI, Amer. Math. Soc (2006)
37. Tsuchida, E., Tsukada, M.: Electronic-structure calculations based on the finite-element method. Phys. Rev. B. 52, 5573–5578 (1995)
38. White, S.R., Wilkins, J.W., Teter, M.P.: Finite-element method for electronic structure. Phys. Rev. B. 39, 5819–5833 (1989)
39. Wohlever, J.C.: Some computational aspects of a group theoretic finite element approach to the buckling and postbuckling analyses of plates and shells-of-revolution. Comput. Methods Appl. Mech. Eng. 170, 373–406 (1999)
40. Xia, F., Chen, H., Song, L., Shen, W.: Design and implementation of numerical simulation mesh data model. J. Comput. Res. Develop. 46((Supp. 1)), 258–264 (2009). (in Chinese)
41. Zhang, D., Shen, L., Zhou, A., Gong, X.: Finite element method for solving Kohn-Sham equations based on self-adaptive tetrahedral mesh. Phys. Lett. A. 372, 5071–5076 (2008)
42. Zienkiewicz, O.C., Taylor, R.L.: The Finite Element Method for Solid and Structural Mechanics, 6th edn. Elsevier, London (2005)
43. Zingoni, A.: Group-theoretic exploitations of symmetry in computational solid and structural mechanics. Int. J. Numer. Methods Eng. 79, 253–289 (2009)