Application of Geometric Eigensubspace Framework in The Characterization of Atomic Structure

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Abstract. The specific atomic structure of materials plays an important role in solid-state physics and materials science because it is inherently related to many physical properties of materials. Various structural fingerprints have been proposed to identify the configuration of atoms. They do not depend on the coordinate system and the order of atoms, so they are more convenient than traditional atomic coordinates. They are unique, but they cannot fully describe the structure of the atom. Therefore, we hope to have a notation that uniquely identifies the atomic configuration and contains as much structural information as possible. This paper proposes a novel and intrinsic representation of atomic structure. We first proposed an extended distance matrix to describe the atomic structure of the cluster. It is different from the traditional distance matrix in that the zero of the diagonal element is replaced with the characteristic quantity of each atom to distinguish different elements. The extended distance matrix contains all the structural information of the cluster. In addition to the overall chirality, through spectral decomposition, the position information of the atoms can be discussed based on the eigenvector coordinate system and the eigensubspace framework. Studies have shown that due to the difference in the number of bonds, the $\Lambda_{dec}$ distance between the diamond atom (the number of bonds is 4) and the other two atoms (the number of bonds is 3) is relatively large, about 0.076; graphene atoms and $C_{60}$ atoms the $\Lambda_{dec}$ distance is relatively small, about 0.051.

Key words: Extended Distance Matrix, Eigensubspace Projection Function, Projection Function, EPF Distance.

1. Introduction
In recent decades, many emerging industries have developed vigorously and society is changing with each passing day. Behind all this is inseparable from the development of science and technology and the research and development of new materials. The so-called clever woman can hardly cook without rice, high-performance materials have always been a vital part of modern industry and cutting-edge industries. Different materials have different characteristic properties, mainly including: thermal properties (heat capacity, thermal conductivity, thermal expansion, boiling point, etc.) and chemical properties (catalytic properties, corrosion resistance, etc.). Some properties also involve various characteristics and energy conversion, such as pyroelectricity, piezolectricity, spintronic properties, photoelectric conversion
performance, photothermal conversion performance, etc. These properties of materials are mainly
dominated by the electromagnetic interaction of electrons outside the core, which can be calculated and
predicted under the theoretical framework of quantum mechanics.

People abandon the traditional representation of atomic coordinates and propose many more
convenient atomic structure representation methods, such as structural fingerprints. The structural
fingerprint is a set of invariants obtained according to the atomic structure of the configuration. It does
not change with the selection of the coordinate system and the order of the atoms, and it can easily
characterize the structure. Many types of structural fingerprints or similar atomic structure
characterization methods have been proposed, each with its own advantages and disadvantages; most of
them are embedded in high-throughput calculation or structure prediction software, which greatly
improves their efficiency. This article will briefly introduce the traditional representation of atomic
coordinates and some atomic structure characterization methods that have emerged in recent years.

This paper proposes the concept of atomic base vector, and uses atomic structure operators to
describe the atomic structure of clusters in the Euclidean space formed by atomic base vectors. Carrying
out the eigenvalue decomposition of the atomic structure operator, we get the eigencoordinates of the
atomic basis vector, which accurately describes the position of the atomic basis vector in Euclidean
space. From the eigencoordinates, we refined a set of invariant eigensubspace projection order (EPA)
of the atom, and combined with its geometric meaning, we derived a more vivid eigensubspace
projection function (EPF). The EPF of an atom subtly reflects the configuration of the surrounding
atomic structure, and the EPF of all atoms constitutes the configuration of the EPF atomic structure
characterization. Based on this characterization method, we also proposed the EPF distance between
configurations to measure the difference in their atomic structure.

2. The Study of Geometric Eigensubspace Framework in The Characterization of Atomic
Structure

2.1. Extended Distance Matrix

Based on previous research on the characteristic roots of the distance matrix, this paper describes the
graph class with a characteristic root multiplicity of \( n - 2 \) in the distance matrix. First, the integerity of
the characteristic root is proved; the diameter of the graph class is obtained by further analysis Is 2;
finally, further characterize the graph class to obtain the specific structure of the graph class [1-2]. Next,
let's look at a few important lemmas:

Let matrix \( A \) be a real symmetric matrix of order \( n \), and its characteristic roots are arranged in non-
increasing order as \( \lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A) \). Let \( M \) be the principal matrix of matrix \( A \) \( m \) (order) \( m \leq n \), the characteristic roots of matrix \( M \) are arranged in non-increasing order as \( \lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_m(M) \), then:

\[
\lambda_i(A) \geq \lambda_i(M) \geq \lambda_{i+n-m}(A)
\] (1)

Where \( 1 \leq i \leq m \).

Let \( A \) be a real symmetric matrix of order \( n \), the largest eigenvalue of matrix \( A \) is denoted as \( \lambda \), matrix
\( M \) is a sub-matrix of matrix \( A \) \( m \times m \). If \( \lambda \) is also an eigenvalue of matrix \( M \), its corresponding
eigenvector is \( X = (x_1, \ldots, x_m)^T \). Then \( X^* = (x_1, \ldots, x_m, 0, \ldots, 0)^T \) is an eigenvector of the matrix \( A \)
corresponding to the atom of \( \lambda \)

2.2. The Eigen-Subspace Projection Order

The eigen-coordinates and the eigen-subspace projection order have their own advantages and
disadvantages in characterizing the geometric position of atoms: the eigen-coordinates accurately
describe the position of the atomic base vector in Euclidean space, but it is based on the eigen The vector
coordinate system will change with the selection of the eigenvector coordinate system; the
eigensubspace projection order is a set of invariants, reflecting the relative position of the atom in the
molecule, but it is not enough to accurately determine the position of the atomic basis vector [3-4]. In
fact, all the structural information of the extended distance matrix $D$ projected in the eigensubspace corresponding to $\lambda_k$ is contained in its projection matrix:

$$P_{\lambda_k} = \sum_{m} p_{m,\lambda_k} p_{m,\lambda_k}^T$$

Among them, $p_{m,\lambda_k}$ is a complete set of eigenvectors corresponding to $\lambda_k$, and they form a set of orthonormal bases of the eigensubspace. $P_{\lambda_k} e_i$ can be used to obtain the projection of each atomic basis vector in the eigen subspace (based on the atomic basis vector coordinate system). Since the projection matrix is symmetric and idempotent, there are:

$$(P_{\lambda_k} e_i)^T (P_{\lambda_k} e_j) = e_i^T P_{\lambda_k}^T P_{\lambda_k} e_j = e_i^T P_{\lambda_k} e_j = e_j^T P_{\lambda_k} e_i$$

It can be seen that the matrix element in the $i$th row and the $j$th column of $P_{\lambda_k}$ is actually the inner product of the projection of the atom $i$ and the atom $j$ in the intrinsic subspace. That is, the diagonal element of $P_{\lambda_k}$ stores the mode of each atom's projection in the eigen-subspace, and the non-diagonal element stores the angle between the projections of each atom. From this perspective, the eigensubspace projection sequence only stores the modes of each atom's projection, and discards the complicated angle relationship between them. In this way, the overall relationship of all atoms is removed, and the problem is only examined from the perspective of a single atom. Therefore, the eigensubspace projection order is only related to the relative position of the atoms [5-6]. Without the angle relationship of the projection, we cannot directly reconstruct the specific configuration of the cluster based on the eigenvalue and the eigensubspace projection order of each atom, and it is even difficult to prove that they can uniquely determine the cluster. However, the contrast eigencoordinates reflect the absolute position of the atom.

2.3. EPF Configuration Space and Its Application

In our EPF atomic structure characterization method, each atom is described by its EPF function, which reflects the configuration of the surrounding atomic structure. The EPFs of all atoms form an intrinsic structural representation of the cluster [7-8]. In other words, an $n$-atom cluster is in an $n$-dimensional configuration space, and each dimension of the space is described by an EPF function, which is called the EPF configuration space. In real three-dimensional space, the coordinates of an atom describe its absolute position in space; and in EPF configuration space, the EPF of an atom describes its structural environment and reflects its relative position in the cluster.

Therefore, the EPFs of atoms influence each other: a slight movement of an atom will not only affect its own EPF, but also the EPFs of surrounding atoms. All EPFs form a whole and together describe the atomic structure of the cluster. In practical applications, we can project multiple clusters into the EPF configuration space, which not only helps us understand the structural relationship between them, but also has many practical applications [9-10]. For example, the potential energy surface of the configuration plays an important role in the global search, structure prediction, transition state, and transition path search. If you can explore the potential energy surface of the configuration as much as possible, you can summarize its laws and characteristics, and design more Targeted and more efficient search methods.

3. Experimental Study of Geometric Eigensubspace Framework in The Characterization of Atomic Structure

3.1. Method Promotion

Whether for clusters or crystals, we can obtain the attenuation distance matrix and the minimum distance matrix. Among them, the attenuation distance matrix corresponds to a certain atom, and each atom has its own attenuation distance matrix, which describes the atomic structure within the $r_{cut}$ range of the atom. The minimum distance matrix corresponds to a set of non-trivial atoms, and they share the same minimum distance matrix, which describes the geometric relationship between the pair of atoms (under translational symmetry). These two matrices do not depend on the selection of the unit cell and the position of the atoms in the unit cell, so they are suitable for structure identification and comparison.
3.2. Practical Application
This article presents several allotrope structures of carbon, namely: graphene, graphite, diamond, zigzag carbon nanotubes, armrest carbon nanotubes and C60. Here, the two types of carbon nanotubes choose single-walled zigzag carbon nanotubes and (handrail-shaped carbon nanotubes). Their diameters are very close, which is convenient for structural comparison. Because the atoms with equivalent relative positions have exactly the same EPF function, so here we only discuss atoms with unequal positions, there are a total of 7. Because these structures are highly symmetrical, most of them only have one type of atoms with unequal positions, except for graphite. Graphite has two types of positions Non-equivalent atoms are derived from the difference in the structure of the outer layer: one type is located at the top position of an atom in the adjacent atomic layer, and the other type is located in the center of the hexagonal vacancy in the adjacent atomic layer.

4. Experimental Research and Analysis of Geometric Eigensubspace Framework in The Characterization of Atomic Structure

4.1. Structural Comparison of Carbon Allotropes
As can be seen in the key mark matrix of graphite and diamond, their key mark matrices are very different, demonstrating the effectiveness of the key mark matrix in identifying different structures. The Euclidean distance monotonously increases with the degree of deformation, reflecting the ability of the key-mark matrix to measure structural similarity. The key logo matrix is embedded in the CALYPSO software to eliminate similar structures. The experiment is shown in Table 1.

| Number of atoms in the system | 14 | 25 | 34 | 49 |
|------------------------------|----|----|----|----|
| Generations                  | 14 | 17 | 23 | 74 |
| To eliminate similar structures | 9  | 18 | 42 | 115 |

Table 1 uses TiO2 as an example to show how this method improves search efficiency. Obviously, it can be seen that eliminating similar structures, CALYPSO only needs fewer steps to search for the most stable configuration. This technique can avoid many repetitive or similar structure calculations, thereby improving the convergence efficiency of the global structure search.

Through our method, the $A^{dec}$ function and $A^{min}$ function of these seven atoms can be obtained. When constructing the attenuation distance matrix, we take the cutoff radius as 10A. In addition, because there is only one kind of atom, we take all the diagonal elements of the matrix as 0. If the diagonal element of the matrix is taken as carbon's atomic number 6, then the EPF function of all atoms will be shifted up by 6 units, which makes no essential difference. Let's analyze their EPF function.

Figure 1. The structures of several allotropes of carbon and the eigensubspace projection functions of their atoms
Figure 1 shows the $\Lambda^{dec}$ function of graphene, diamond and $C_{60}$ atoms. The structures of these three carbon allotropes are quite different from each other. Among them, graphene is a two-dimensional crystal, its atoms form bonds with three surrounding atoms; diamond is a three-dimensional crystal, its atoms form bonds with four surrounding atoms; $C_{60}$ is a zero-dimensional cluster, and its atoms form bonds with three surrounding atoms. But unlike graphene, these atoms are not on the same plane and the bond angles are also different. It can be seen from the figure that the $\Lambda^{dec}$ functions of these three configurations of atoms are very different, reflecting the differences in their structures. The dec $d$ distances of these three atoms are also shown in the figure. Due to the difference in the number of bonds, the $\Lambda^{dec}$ distance between the diamond atom (the number of bonds is 4) and the other two atoms (the number of bonds is 3) is relatively large, about 0.076; the $\Lambda^{dec}$ distance between graphene atoms and $C_{60}$ atoms is relatively small, about 0.051.

5. Conclusion
This paper presents the $\Lambda^{min}$ function of graphene and two kinds of carbon nanotube atoms. The two types of carbon nanotubes have similar diameters and similar atomic structures in the distance, so they have similar $\Lambda^{min}$ functions. In contrast, graphene has a two-dimensional structure. From the perspective of large size and lattice, it has no structural similarity with carbon nanotubes, so it has a very different $\Lambda^{min}$ function. This can also be reflected quantitatively by their $d^{min}$ distance.

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