Tips in the first principles electronic structure computation: How to determine sample k-points in the Brillouin zone integration with symmetry

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Abstract

In this short notes, we give a concise account of determining sample k-points in the Brillouin zone integration, where we should consider the symmetry of the crystal. The procedure is represented by the pseudo-code.

1 Introduction

In the first principles electronic structure calculation for the periodic system we have to execute the numerical integration in the wave-number space: the integration in the Brillouin zone as follows,

$$\int f(k_x, k_y, k_z) dk_x dk_y dk_z. \quad (1)$$

The integral is actually replaced by the summation on the discrete sample points:

$$\sum w_i f(k_x^i, k_y^i, k_z^i), \quad (2)$$

where the summation is taken over the sampling points (k_x^i, k_y^i, k_z^i) with weight w_i [1]. As the periodic structure is often equipped with the symmetry, the physical property of a quantum mechanical quantity $f(k)$ on a k-point might be related to that on another k-point $f(R \cdot k)$ by the symmetry operation R ; these two quantities often take the same value. Thus it is practical to compute the quantum mechanical quantity only in the representatives of the sampling k-points, from which we could derive the information on the other sampling k-points. These representatives should be taken in the minimum fragment of the range of the integral: the irreducible Brillouin zone, in which the weights on sampling points may be different. In the following section, we explain how to determine the sampling points in the reduced Brillouin zone and how to put the weights on them.

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2 Algorithm

We use the following notation.

The wave-number vector is given by the coefficients (k_1, k_2, k_3) on the reciprocal lattice vectors (B_1, B_2, B_3) :

$$K = k_1 \cdot B_1 + k_2 \cdot B_2 + k_3 \cdot B_3. \quad (3)$$

(The reciprocal vector is related to the crystal primitive vectors (A_1, A_2, A_3) in the standard way : $A_i \cdot B_i = \delta_{i,j}$.)

The symmetry operations are represented by a 3×3 matrices. For the simplicity of the algorithm, they are represented by the matrix operation of the threefold tuple of the coefficients (k_1, k_2, k_3) :

$$R \cdot (k_1, k_2, k_3)^t. \quad (4)$$

It is an easy task to obtain this matrix by the linear algebra.

2.1 Generation of uniform k-points

We distribute uniformly the sample k-points in the whole Brillouin zone:

$$k_1^{(i,j,l)} = \frac{(i-1) + s_1}{N_1}, \quad (5)$$

$$k_2^{(i,j,l)} = \frac{(j-1) + s_2}{N_2}, \quad (6)$$

$$k_3^{(i,j,l)} = \frac{(l-1) + s_3}{N_3}, \quad (7)$$

where N_1 , N_2 , and N_3 are the numbers of divisions along each reciprocal vector; (s_1, s_2, s_3) are the shift of the origin. If we do not assume any symmetry, the algorithm ends here. The generated k-points are now stored in the array U. The weight for each k-point is taken to be $\frac{1}{N_1 N_2 N_3}$.

2.2 Removal of unnecessary sampling points (reduction to irreducible zone)

Let S be the k-points in the irreducible zone; they will be culled out of the uniform sample k-points U. Let R be the set of symmetry operations; it includes operations $R(j)$, $j=1, \dots, NT$.

Initialization:

Set $S=\{ \}$ (an empty set).

Give the index to the elements $k(i)$ in U as $i=1, \dots, N$.

The weight for each element is $w(i)=1/(N_1*N_2*N_3)$.

Give the boolean marker to $k(i)$: $related(i) = .FALSE$.

The index N to the element $(k_1^{(i,j,l)}, k_2^{(i,j,l)}, k_3^{(i,j,l)})$ might be given by

$$N = (i-1) * N_3 * N_2 + (j-1) * N_3 + l, \quad (8)$$

so that the tuples of the index are sorted by the lexicographic order. The boolean marker $related(i)$ indicates whether the corresponding k-point is related to the others by the symmetry or not. The algorithm elicits the minimum representative of the related k-points in this order.

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For i=1,N (the first loop)
  Take one sample point k(i) in U.
  If the marker: related(i) == .FALSE., execute the second loop.

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If the previous steps of the loop have proved that $k(i)$ is related to other k -points, we should neglect it in the subsequent consideration. We set $i \rightarrow i + 1$ and begin the next step of the first loop.

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For j =1,NT (the second loop)
  Compute the operation R(j) on k(i) : R(j)*k(i)
  Pull back R(j)*k(i) into the primitive Brillouin zone.
  The computed value is stored at (RK(1), RK(2), RK(3)).

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As aforementioned, the sampling points are given by the coefficients to the reciprocal vectors; those of the elements in the uniform k -points prepared at first lie in the interval $[0, 1]$. After the symmetry operation, however, they might escape from this interval. So by adding or extracting the integer 1, we translate it in the interval $[0, 1]$.

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(Still continues the second loop)
For ip=i+1,N (the third loop)
  CHECK 1:
    Compare (RK(1),RK(2),RK(3))
    with k(ip) = (KIP(1),KIP(2),KIP(3)).
    If they are the same, increase the weight on k(i) :
      w(i) - - > w(i)+ w(ip),
      And set the marker: related(ip) = .TRUE.
      And skip CHECK 2.
  CHECK 2:
    Compare (1-RK(1),1-RK(2),1-RK(3))
    with k(ip) = (KIP(1),KIP(2),KIP(3)).
    If they are the same, increase the weight on k(i) :
      w(i) - - > w(i)+ w(ip)
      And set the marker: related(ip) = .TRUE.

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End of the third loop

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End of the second loop

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End of the first loop

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In the third loop, when CHECK 1 proves that these two vectors are the same, the quantity on $k(ip)$ is retrievable from $k(i)$ and we do not use $k(ip)$ as the representative. In CHECK 2, $(1-RK(1), 1-RK(2), 1-RK(3))$ is the time reversal of $R(j)*k(i)$. If they are the same, the quantity on $k(ip)$ is also retrievable from $k(i)$. In this way, we cull out the irreducible set of the sample k -points and we prepare the suitable weight on each of them.

3 Summary

In this article, we give the pseudo-code of sample k -points in the numerical Brillouin zone integration. Although the algorithm is a simple procedure,

it is hidden behind the old fashioned subroutines in the implementation of first electronic structure computations and we could not comprehend it easily. The authors have comprised this article with the hope that it exonerates the burden of young programmers. In fact, the scheme of the numerical integration through the summable weight on the sample k-points is a rough estimation: in more accurate computation we should employ some kinds of the interpolation, such as the tetrahedron method [2]. However, the generation of sampling points adequate for the crystal symmetry, which is explained in this article, would be useful in more accurate numerical integration.

References

- [1] Monkhorst, Hendrik J. and Pack, James D, “Special points for Brillouin-zone integration”, Phys. Rev. B, Vol. 13, pp 5188–5192, 1976.
- [2] Blöchl, Peter E. and Jepsen, O. and Andersen, O. K., “Improved tetrahedron method for Brillouin-zone integrations”, Phys. Rev. B, vol 49, pp 16223–16233, 1994.