A New Interpretation of Discontinuity Factor

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ABSTRACT

A new interpretation of the discontinuity factor (DF) for scalar flux, partial current, and angular flux is discussed. Conventionally, the DF is considered as the discontinuous condition of scalar flux, partial current, or angular flux at an interface. In the new interpretation, the DF is considered as the "refractive" index of materials for partial current or angular flux that conserves odd-parity or odd-moment angular flux at an interface of different materials. It is related to the transmission and reflection of partial current or angular flux at an interface where different materials adjacent. Using the present interpretation, a fundamental issue of neutron balance (*i.e.*, artificial loss or production of neutrons at an interface due to discontinuous condition), which would appear in the conventional interpretation of DF, can be resolved.

KEYWORDS: Discontinuity factor, scalar flux, partial current, angular flux, refractive index

I. INTRODUCTION

Discontinuity factor (DF) is widely used in reactor physics calculations. Historically, the DF is introduced for the diffusion theory by Koebke [1] and later extended by Smith as the generalized equivalence theory (GET) [2]. In the diffusion theory, the discontinuity (or jump) condition is applied to scalar flux while the continuity condition is used for the net neutron current. By preserving the net neutron current, the neutron leakage from a region is preserved. Thus the reaction rate in a region, which is the most important quantity in reactor physics calculation, is consequently preserved. The DF is additional freedom that is necessary to preserve the reference net current. The scalar flux is expressed as υN where υ and N are neutron velocity and neutron density, respectively. Neutron velocity does not change at the interface unless the neutron experiences collision. Therefore, from the physical point of view, the discontinuity condition for scalar flux seems to be somewhat strange since it means that neutron density is discontinuous at an interface. However, it has been sometimes justified by the following reason – since the scalar flux in a homogeneous geometry is an artificial (not a physical) value thus the physical requirement (continuity of neutron density) is not necessary. Actually, the net current is continuous thus no inconsistency occurs from the viewpoint of neutron balance, which is essential in a neutronics calculation.

The application of DF has been extended from the diffusion theory to transport theory [3]-[10]. In the case of transport theories using the second order differential equations (*i.e.*, the simplified Pn, the Pn, and the even parity transport theories), application of DF can be considered as a straightforward extension of the diffusion theory since even and odd parity angular fluxes (or angular flux moments) correspond to the scalar flux and the net current in diffusion theory, respectively. In other words, in these transport theories, the DF for even parity angular flux (or angular flux moment) can be calculated using the odd parity angular flux (or angular flux moment) as the boundary conditions. Since continuity of the odd parity angular flux (or angular flux moment) is guaranteed, neutron balance (*i.e.*, continuity of net current) at an interface is rigorously preserved.

However, as discussed in the latter section, when the DF is directly applied to the partial current or the angular flux, the situation can be different. These cases would happen when the DF is used in the transport theories using the first order differential equation, *e.g.*, the MOC or the discrete ordinate method. In these cases, the net current can be discontinuous at an interface. It means that neutrons are artificially produced or disappeared at the interface thus neutron balance (preservation of a number of neutrons) at the interface is not guaranteed anymore.

In the present paper, a new interpretation of the DF is discussed. In order to preserve neutron leakage, odd-parity angular flux (or angular moment) should be preserved and thus it should be continuous at an interface. Under this interface condition, the DF for angular flux (or partial current) is considered as the partial reflective boundary condition between different regions, which has the analogy with the reflection of light between different materials. In the present interpretation, angular flux or partial current is partially "reflected" or "transmitted" at an interface without artificial loss or production of neutrons.

In Section 2, a brief review on applications of DF is provided though it is not extensive. Current issues of DF and a new interpretation of DF are discussed in Section 3. Finally concluding remarks are provided in Section 4.

II. APPLICATIONS OF DISCONTINUITY FACTORS

Though an extensive review of the DF is out of the scope of the present paper, major applications of the DF are summarized in this section.

II.A. Scalar Flux and Partial Current in Diffusion Theory

In the diffusion theory, the DF is applied to scaler flux to preserve the net current at a region interface:

$$\begin{aligned} f_L \phi_L &= f_R \phi_R, \\ J_L^{net} &= J_R^{net}, \end{aligned} \tag{1}$$

where

f_L and f_R : DFs for the left and the right region surfaces, respectively,

ϕ_L and ϕ_R : scalar fluxes at the left and the right region surfaces, respectively,

J_L^{net} and J_R^{net} : net currents at the left and the right region surfaces, respectively,

as shown in Fig.1.

Now we consider the relationship between the net and partial currents in diffusion theory [11]:

$$
\begin{aligned}
J_L^{out} &= \frac{1}{4}\phi_L + \frac{1}{2}J_L^{net}, J_L^{in} = \frac{1}{4}\phi_L - \frac{1}{2}J_L^{net}, \\
J_R^{in} &= \frac{1}{4}\phi_R + \frac{1}{2}J_R^{net}, J_R^{out} = \frac{1}{4}\phi_R - \frac{1}{2}J_R^{net}.
\end{aligned}
\tag{2}
$$

Using Eqs.(1) and (2), the relation of partial currents considering the DF is described as:

$$
\begin{aligned}
J_R^{in} &= \frac{2f_L}{f_L + f_R}J_L^{out} + \frac{f_L - f_R}{f_L + f_R}J_R^{out}, \\
J_L^{in} &= \frac{2f_R}{f_L + f_R}J_R^{out} + \frac{f_R - f_L}{f_L + f_R}J_L^{out},
\end{aligned}
\tag{3}
$$

where

J_L^{in} and J_L^{out}: incoming and outgoing partial currents at the left region surface,

J_R^{in} and J_R^{out}: incoming and outgoing partial currents at the right region surface,

as shown in Fig.1.

In this case, the partial currents are discontinuous at the interface as shown in Fig.2 but the net current is continuous since the following relation holds:

$$
J_L^{net} = J_L^{out} - J_L^{in} = J_R^{in} - J_R^{out} = J_R^{net}. \tag{4}
$$

II.B. Partial Current in the Black-Box Homogenization Theory

In the black-box homogenization theory, Sanchez proposed the partial current DF that is applied to the partial current [3]:

$$
\begin{aligned}
f_R^{in}J_R^{in} &= f_L^{out}J_L^{out}, \\
f_L^{in}J_L^{in} &= f_R^{out}J_R^{out}.
\end{aligned}
\tag{5}
$$

The partial current DF is evaluated to preserve the partial current obtained by the reference calculation (usually, based a higher order method using a fine calculation condition). The partial current DF rigorously preserves the net current in the reference condition, which should be continuous. However, in an application (non-reference condition), the partial current DF does not necessarily preserve the net current expressed by partial currents in each region. For example, let us consider the situation of $J_R^{out} = 0$. In this case, $J_L^{in} = 0$ from Eq.(5) thus the net current in each region surface is calculated by:

$$J_L^{net} = J_L^{out} - J_L^{in} = J_L^{out},$$
$$J_R^{net} = J_R^{in} - J_R^{out} = J_R^{in}. \tag{6}$$

When Eq.(5) is considered, it is clear that $J_L^{net} \neq J_R^{net}$ except for $f_R^{in} = f_L^{out}$, which is not generally satisfied. In order to make the net current continuous at an interface, the corrected partial currents (*i.e.*, $f_R^{in} J_R^{in}$, $f_L^{out} J_L^{out}$, $f_L^{in} J_L^{in}$, $f_R^{out} J_R^{out}$) should be used for the neutron balance calculation in each region.

II.C. Even and Odd Angular Flux Moments in Pn Theory

Let us consider the Pn transport equation in a one-dimensional slab geometry for simplicity. In this case, the Pn equation has a similar form with that of the diffusion theory [11][12]. Therefore, the concept of DF in the diffusion theory can be applied in a straightforward manner [5]. Namely, the DF can be applied as follows:

$$f_{2n,L}\phi_{2n,L} = f_{2n,R}\phi_{2n,R},$$
$$\phi_{2n+1,L} = \phi_{2n+1,R}, \tag{7}$$

where

n: the order of Pn expansion coefficient, integer ($n \geq 0$),

$f_{2n,L}$ and $f_{2n,R}$: DFs for the even angular flux moments at the left and the right surfaces,

$\phi_{2n,L}$ and $\phi_{2n,R}$: even angular flux moments at the left and the right surfaces,

$\phi_{2n+1,L}$ and $\phi_{2n+1,R}$: odd angular flux moments at the left and the right surfaces.

Actually, Eq.(7) is a generalization of Eq.(1) since the scalar flux and the net current are the 0th and 1st order angular moments in the Pn theory, respectively. When Eq.(7) is used, the net current is preserved since $J_L^{net} = \phi_{1,L} = \phi_{1,R} = J_R^{net}$ though even angular flux moments are discontinuous.

II.D. Even-Parity Angular Flux

The transport equation for the even-parity angular flux has the similar form with the diffusion equation. Therefore, DF for the diffusion theory can be directly applied [5][6][9]:

$$\begin{aligned} f_L^e(\mathbf{\Omega})\psi_L^e(\mathbf{\Omega}) &= f_R^e(\mathbf{\Omega})\psi_R^e(\mathbf{\Omega}), \\ \psi_L^o(\mathbf{\Omega}) &= \psi_R^o(\mathbf{\Omega}), \end{aligned} \tag{8}$$

where

$f_L^e(\mathbf{\Omega})$ and $f_R^e(\mathbf{\Omega})$: DFs for even-parity angular flux at the left and the right surfaces for direction $\mathbf{\Omega}$, and $f_L^e(\mathbf{\Omega}) = f_L^e(-\mathbf{\Omega})$, $f_R^e(\mathbf{\Omega}) = f_R^e(-\mathbf{\Omega})$.

$\psi_L^e(\mathbf{\Omega})$ and $\psi_R^e(\mathbf{\Omega})$: even-parity angular fluxes at the left and the right surfaces for direction $\mathbf{\Omega}$,

$\psi_L^o(\mathbf{\Omega})$ and $\psi_R^o(\mathbf{\Omega})$: odd-parity angular fluxes at the left and the right surfaces for direction $\mathbf{\Omega}$.

The even and odd parity angular fluxes are defined by:

$$\begin{aligned} \psi_L^e(\mathbf{\Omega}) &= \frac{\psi_L(\mathbf{\Omega}) + \psi_L(-\mathbf{\Omega})}{2}, \\ \psi_L^o(\mathbf{\Omega}) &= \frac{\psi_L(\mathbf{\Omega}) - \psi_L(-\mathbf{\Omega})}{2}, \\ \psi_R^e(\mathbf{\Omega}) &= \frac{\psi_R(\mathbf{\Omega}) + \psi_R(-\mathbf{\Omega})}{2}, \\ \psi_R^o(\mathbf{\Omega}) &= \frac{\psi_R(\mathbf{\Omega}) - \psi_R(-\mathbf{\Omega})}{2}, \end{aligned} \tag{9}$$

where $\psi_L(\mathbf{\Omega})$ and $\psi_R(\mathbf{\Omega})$ are the angular flux at the left and the right surfaces for direction $\mathbf{\Omega}$, respectively.

Using Eqs.(8) and (9), the relation of angular fluxes considering DF can be written by:

$$\begin{aligned} \psi_R(\mathbf{\Omega}) &= \frac{2f_L^e(\mathbf{\Omega})}{f_L^e(\mathbf{\Omega}) + f_R^e(\mathbf{\Omega})}\psi_L(\mathbf{\Omega}) + \frac{f_L^e(\mathbf{\Omega}) - f_R^e(\mathbf{\Omega})}{f_L^e(\mathbf{\Omega}) + f_R^e(\mathbf{\Omega})}\psi_R(-\mathbf{\Omega}), \\ \psi_L(-\mathbf{\Omega}) &= \frac{2f_R^e(\mathbf{\Omega})}{f_L^e(\mathbf{\Omega}) + f_R^e(\mathbf{\Omega})}\psi_R(-\mathbf{\Omega}) + \frac{f_R^e(\mathbf{\Omega}) - f_L^e(\mathbf{\Omega})}{f_L^e(\mathbf{\Omega}) + f_R^e(\mathbf{\Omega})}\psi_L(\mathbf{\Omega}). \end{aligned} \tag{10}$$

As shown in Fig.3, angular fluxes are discontinuous at the interface but odd-parity angular flux is continuous due to Eq.(8). Since the net current is the solid angle integration of the odd-parity angular flux multiplied by direction cosine, it is also continuous at the interface. The scalar flux is discontinuous at the interface since even-parity angular flux is discontinuous. Equation (10) can be directly used for MOC though it is derived based on the interface conditions for the odd- and even-parity angular fluxes. However, use of Eq.(10) poses an implementation issue in MOC since the forward and backward angular fluxes are entangled at the interface. [9]

II.E. Angular Flux

The DF can be directly applied to the angular flux, which is the angular flux DF [4][7][10].

$$\begin{aligned} f_R^{af}(\mathbf{\Omega})\psi_R(\mathbf{\Omega}) &= f_L^{af}(\mathbf{\Omega})\psi_L(\mathbf{\Omega}), \\ f_L^{af}(-\mathbf{\Omega})\psi_L(-\mathbf{\Omega}) &= f_R^{af}(-\mathbf{\Omega})\psi_R(-\mathbf{\Omega}). \end{aligned} \tag{11}$$

This treatment is similar to the partial current DF appeared in the black-box homogenization theory. In the reference condition, angular flux is rigorously preserved since the reference angular flux (continuous at the interface) is reproduced by the angular flux DF. However, in a non-reference condition (*e.g.*, a variation of boundary condition, colorset geometry), preservations of the odd-parity angular flux as well as the net current using the uncorrected angular fluxes are not guaranteed. In a simple case, let us consider the situation $\psi_R(-\mathbf{\Omega}) = 0$. In this case, $\psi_L(-\mathbf{\Omega}) = 0$ from Eq.(11) thus the odd parity angular flux is calculated by:

$$\begin{aligned} \psi_L^o(\mathbf{\Omega}) &= \frac{\psi_L(\mathbf{\Omega}) - \psi_L(-\mathbf{\Omega})}{2} = \frac{\psi_L(\mathbf{\Omega})}{2}, \\ \psi_R^o(\mathbf{\Omega}) &= \frac{\psi_R(\mathbf{\Omega}) - \psi_R(-\mathbf{\Omega})}{2} = \frac{\psi_R(\mathbf{\Omega})}{2}. \end{aligned} \tag{12}$$

When Eq. (11) is considered, it is clear that $\psi_L^o(\mathbf{\Omega}) \neq \psi_R^o(\mathbf{\Omega})$ except for $f_R^{af} = f_L^{af}$, which is not generally satisfied. Similar to the partial current DF, corrected angular fluxes (*i.e.*, $f_R^{af}(\mathbf{\Omega})\psi_R(\mathbf{\Omega})$, $f_L^{af}(\mathbf{\Omega})\psi_L(\mathbf{\Omega})$, $f_L^{af}(-\mathbf{\Omega})\psi_L(-\mathbf{\Omega})$, $f_R^{af}(-\mathbf{\Omega})\psi_R(-\mathbf{\Omega})$) should be used to calculate the net current at the interface to make the net current at continuous. In order to avoid this issue, Eq.(10) can be used instead, but the implementation issue described in the previous section should be addressed.

III. AN INTERPRETATION OF DISCONTINUITY FACTOR FOR ANGULAR FLUX AND PARTIAL CURRENT

In the all definitions of DF described in section 2, the angular flux, as well as the partial current, are discontinuous at an interface of regions. The angular flux or the partial current represents a stream of neutrons in a particular direction. Thus, in principle, any discontinuity of angular flux at an interface would cause artificial neutron loss or production at the interface. It can be justified since the angular flux or the partial current at the "homogenized" region is an artificial (not physical value). However, in this section, we will introduce alternate interpretation for DF in order to address this issue.

In the following discussion, we will focus on the DF appeared in the diffusion (Eq.(1)), the Pn, the simplified Pn (Eq.(7)), and the even parity (Eq.(8)) theories. The DFs appeared in the black-box homogenization (Eq.(5)) and the angular flux (Eq.(11)) are not included in the following discussion.

In an ideal correction, all angular fluxes (or angular moments) should be continuous and be identical to the reference values at the interface. However, in practice, we cannot realize such a condition using a coarse calculation condition. Therefore, we consider an interface condition in which weighted integrals of angular flux over an angular space are continuous. Here, we can choose the range of integration for angular space. When the range of integration for angular space is smaller, the performance of the correction would be better. The smallest range corresponds to the odd-parity angular flux (Eq.(8)) that sums angular fluxes only for the forward and backward directions. Contrary, the largest range corresponds to the net current (Eq.(1)), which integrates all direction considering the direction cosine. These corrections can be used to capture discrepancy between two different calculations, *e.g.*, diffusion versus transport, homogeneous versus heterogeneous, and coarse versus fine calculation conditions.

When the interface conditions of Eqs.(1) and (8) are considered, Eqs.(3) and (10) are obtained for the partial currents and the angular fluxes as described in the previous section. By a physical insight, the "transmission" and the "reflection" coefficients for the partial current and the angular flux going from the left region to the right region are defined as follows:

$$\begin{gathered}\text{Transmission coefficient for partial current:}\,\frac{2f_L}{f_L+f_R},\\ \text{Reflection coefficient for partial current:}\,\frac{f_R-f_L}{f_L+f_R}.\end{gathered} \tag{13}$$

$$\begin{gathered}\text{Transmittion coefficient for angular flux:}\,\frac{2f_L^e(\mathbf{\Omega})}{f_L^e(\mathbf{\Omega})+f_R^e(\mathbf{\Omega})},\\ \text{Reflection coefficient for angular flux:}\,\frac{f_R^e(\mathbf{\Omega})-f_L^e(\mathbf{\Omega})}{f_L^e(\mathbf{\Omega})+f_R^e(\mathbf{\Omega})}.\end{gathered} \tag{14}$$

The similar transmission and reflection coefficients are defined for the partial current and the angular flux going from the right region to the left region.

An important point of the transmission and the reflection coefficients is that the sum of these coefficients is automatically 1. Therefore, the partial current or the angular flux is "transmitted" or "reflected" at an interface thus there is no artificial loss or production of the partial current or the angular flux. It should be noted that the transmission or reflection of the partial current or the angular flux mentioned above is not a physical phenomenon. It is a mathematical interface condition thus it should be distinguished from the conventional (*i.e.*, realistic and physical) transmission and reflection coefficients for neutrons that are traditionally defined in a volumetric region.

The discussion so far suggests that there is an alternative mathematical approach to derive DF. Namely, we can start the transmission and reflection coefficients for the partial current or the angular flux to derive DF. In this approach, continuity of odd-parity angular flux (or net current) is guaranteed while even-parity angular flux (or scalar flux) becomes discontinuous at an interface. It should be noted that the present concept can be applied not only to the partial current or the angular flux but also to other quantities that can be obtained by integration of angular flux in a partial angular space.

Without heterogeneity, the transmission and the reflection coefficients are normally 1 and 0 at an interface, respectively. In this case, the partial current or the angular flux is continuous at an interface. Contrary, when the transmission and the reflection coefficients are not 1 and 0, respectively, part of the partial current or the angular flux is reflected at the interface, which makes the scaler flux, the partial current, or the angular flux discontinuous.

An analogy of this phenomena is the refraction index of light. The light is split into the transmitted and the reflected lights at a material interface. As shown Fig.4, the light of amplitude A is entering the interface from the left side along with the normal direction of the interface. In this case, the amplitudes of the transmitted and reflected lights (for the p-polarization) are given by Eq.(15) [13].

$$\begin{aligned} A_t &= \frac{2n_L}{n_L + n_R} A, \\ A_r &= \frac{n_R - n_L}{n_L + n_R} A, \end{aligned} \tag{15}$$

where

n_L and n_R: refractive indexes for the left and the right materials,

A, A_t, and A_r: amplitude of entering, transmitted, and reflected lights.

There is clear similarity among Eqs.(13), (14) and (15) as follows:

$$n_L \leftrightarrow f_L^e(\boldsymbol{\Omega}),$$
$$n_R \leftrightarrow f_R^e(\boldsymbol{\Omega}), \quad (16)$$
$$A \leftrightarrow \psi_L(\boldsymbol{\Omega}).$$

The reflection of light happens at the interface where different materials are adjacent, *i.e.*, the refractive indexes of adjacent materials are different. This is a very good analogy for neutronics calculation. When different materials having different neutronics properties are adjacent, the "reflection" of angular flux (or partial current) occurs at the interface, which is expressed by the DF. In this sense, the DF can be related to the transmission and reflection condition of angular flux (or partial current) at the material interface rather than the simple discontinuous condition. It should be again noted that the "reflection" is an artificial one and is not a physical phenomenon. In the case of diffusion theory, the DF can be related to the transmission and reflection conditions of partial current. By adopting the present physical interpretation, unphysical interpretation for scalar flux (discontinuity of neutron density) is no more necessary.

It should be noted that the "reflection" of angular flux would be different from the actual reflection (*e.g.*, that at a reflective boundary). In actual reflection, the direction of neutron changes according to the reflection angle. However, in the present case, the opposite direction is used after reflection.

In the conventional sense, the transmission and reflection coefficients take the value of [0, 1]. However, the transmission coefficient appeared in Eqs.(13) and (14) can be larger than 1 and the reflection coefficient can be negative when DF can take any positive value. This seems somewhat strange in the analogy of light. Let us consider neutrons traveling from left to right. When the transmission coefficient is less than 1 (*e.g.*, $f_L < f_R$), the right region tends to "reject" entering neutrons from the left region thus partial reflection occurs. Contrary, the transmission coefficient larger than 1 (*e.g.*, $f_L > f_R$), the right region requires more neutrons from the left region or the left region tends to "push out" neutrons to the right region. The additional (or excess) neutrons provided from the left region to the right region are offset by the reflected negative partial current or the angular flux. Of course, other physical pictures can be considered as an interpretation of the present approach.

IV. CONCLUSIONS

A new interpretation of the discontinuity factor (DF) is discussed. In the present interpretation, DF is considered as an index that is related to the transmission and the reflection of angular flux or partial current at a region interface. The discontinuity of scalar flux, partial current, or angular flux is can be considered based on this concept. Based on the present interpretation, unphysical interpretation (*e.g.*, discontinuity of neutron density at an interface) is not necessary. Furthermore, derivation of alternate DF would be possible using the present concept, which utilizes the concept of artificial transmission and reflection at an interface.

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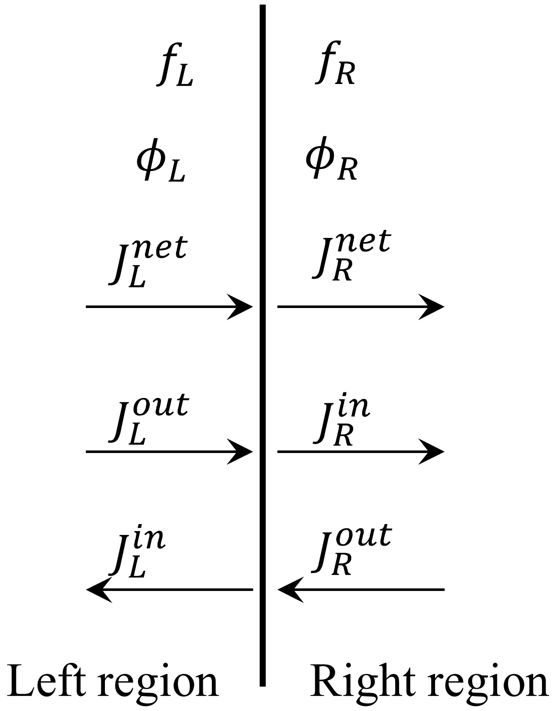

Fig.1 DF and definitions of related quantities

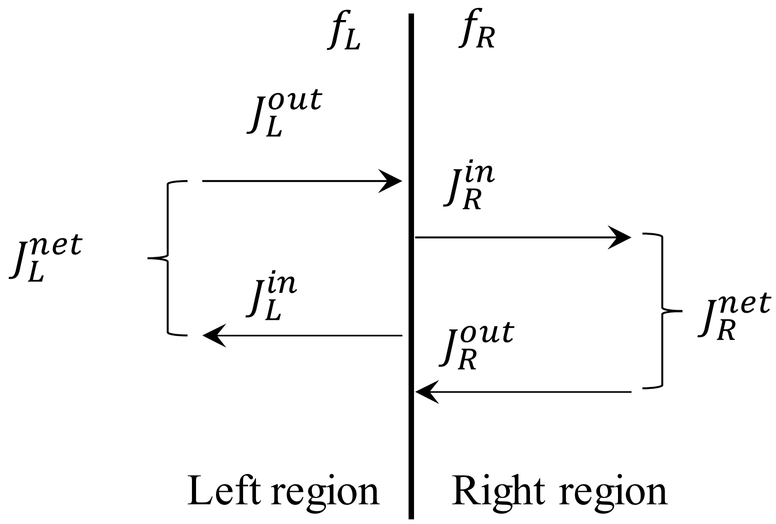

Fig.2 DF and partial currents

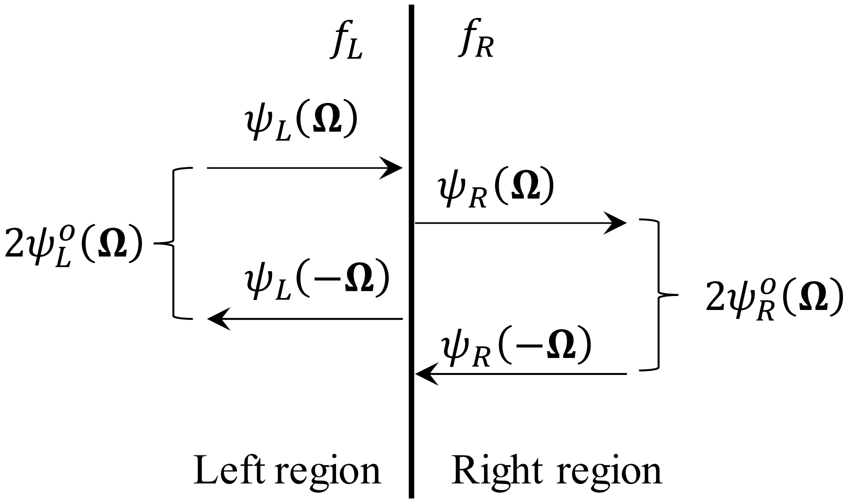

Fig.3 DF and angular fluxes

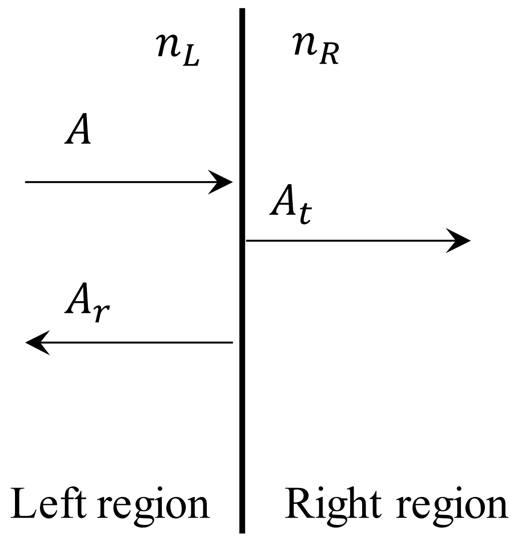

Fig.4 Transmission and reflection of light entering from the left side