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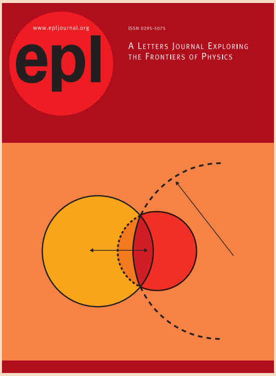
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Quantitative analysis method for extraordinary optical transmission of thin microcavity by the catastrophic theory

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Abstract – Extraordinary optical transmission (EOT) can be regarded as a phase transition process based on the variation of the aperture of the thin microcavity by the published results. Considering that the catastrophe theory could describe quantitatively any phase transition process, a novel method is proposed to analyze the EOT transition quantitatively based on a cusp catastrophic model with dimensionless analysis. The quantitative relationship of transmitted energy spectral density is fully obtained, which is also related to the aperture radius and incident electromagnetic frequency. Furthermore, from this method, a quantum transition factor is derived strictly to describe the EOT transition process, which can be divided into wave region, wave-particle duality region and quantum region with the factor increasing from 0 to 1, and Bethe's aperture theory stating that transmission is proportional to $(r/\lambda)^4$ is only one of our special cases in the wave region. Finally, the influence of the aperture and the frequency of incident wave on the EOT transmittance is analysed, and the catastrophic model is verified by previous experiments. The novel method of transition analysis provides a new insight into the EOT.

Introduction. – Ebbesen and co-workers demonstrated the phenomenon of extraordinary optical transmission (EOT) through the metallic film with an array of subwavelength holes in 1998 [1], which was surprising because Bethe's aperture theory predicts the transmission is proportional to $(r/\lambda)^4$ [2], where r is the thin microcavity radius and λ is the incident wavelength, therefore, the transmission is negligible through the thin microcavity. EOT represents the phenomenon that the transmission shows an enhancement of several orders of magnitude with respect to the classical aperture theory, its intriguing physical properties have attracted tremendous attention. Lots of experimental and theoretical investigations have been carried out on EOT in the past decades [3–6]. Recently, EOT phenomenon has been used in filter sensing and detection design widely. In order to guide the design of related devices effectively, there has been great interest to investigate the physical mechanism behind this effect.

First theories about EOT claimed the key role of surface plasmons (SPP) [7]. However, the same phenomenon was also discovered in some metals with positive real part of the permittivity, and EOT has also been successively observed in THz [8], which contradicts the physical mechanism of SPP. Surface Bloch modes (SBMs) were reported to explain EOT [9], which can enhance the electromagnetic field on the metal surface, thus enhancing the light transmitted into the subwavelength hole array. Nevertheless, Qiu [10] proved that EOT is mainly determined by the aperture size and almost independent of the periodicity, and also attributed the mechanism of EOT to localized surface plasmon (LSP). In addition, CDEW [11] (composite diffraction evanescent waves) and HW [12] (hybrid wave) are also used to explain the EOT phenomenon.

Catastrophe theory is a branch of differential manifold topology and singularity theory, which can explain the phenomenon of gradual quantitative change to sudden qualitative change. Any system from one phase to another can be described by 7 types of elementary catastrophe models with the corresponding different potential functions based on Thom's theory. In some previous papers, Liang *et al.* [13–16] proposed a general non-equilibrium phase transition process to analyze the turbulence transition, which has been applied to explain the sound absorption of porous materials. Wu [17] introduced a novel kind of equations linking the quantum dynamics and the

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classical wave motions. In general, the catastrophe theory can provide a new understanding of EOT from the perspective of phase transition.

In this paper, the extraordinary optical transmission (EOT) can be regarded as a phase transition process based on the variation of the aperture of the thin microcavity by the published results. The cusp catastrophe model is selected and the quantitative description of EOT transition is achieved by dimensionless analysis. Accordingly, the quantitative relationship of transmitted energy spectral density is fully obtained, which is also related to the aperture radius and incident electromagnetic frequency. Besides, a quantum transition factor is derived strictly to describe the EOT transition process, which can be divided into wave region, wave-particle duality region and quantum region with the factor increases from 0 to 1. Importantly, the fact that transmission is proportional to $(r/\lambda)^4$ in the wave region is only one of our special cases, which also verifies the accuracy of our theory. Finally, the influence of the aperture and the frequency of incident wave on the EOT transmittance is analyzed, and the catastrophic model is verified by previous experiments.

Quantitative analysis method for EOT based on a cusp catastrophe model. – Based on our previous research [18,19], we demonstrate that the EOT of the thin microcavity is generally attributed to the macroscopic quantum effects. A critical radius R_0 is found in the thin microcavity under a certain incident electromagnetic wavelength. The whole EOT process, with the aperture radius r varying, can be divided into three regimes: macroscopic quantum region ($R < R_0/2$), wave-particle duality region ($R_0/2 < R < R_0$) and wave region ($R > R_0$). In macroscopic quantum region, the edge field enhancement phenomenon is prominent in the transmitted field, and EOT phenomenon emerges. In wave-particle duality region, edge effect and near-field diffraction phenomenon exist simultaneously. In wave region, field edge effect disappears and prominent near-field diffraction fringes appear in the transmitted field, the corresponding EOT also disappears. Thus, the cusp catastrophic model can be used to quantitatively describe the transition of the three state regimes. Figure 1(a) shows the equilibrium surface of the cusp catastrophic model with two control variables. Figure 1(b) shows the non-equilibrium phase transition path with three system phases and two phase transition points.

The potential function of cusp catastrophe model with aperture radius r as independent variable is:

$$V(r) = r^4 + mr^2 + nr. \tag{1}$$

The governing equation of fold catastrophe model can be expressed as follows:

$$4r^3 + 2mr + n = 0, \tag{2}$$

where m and n are the key parameters determining the phase transition process, which are composed by a variety of physical parameters. According to the macroscopic quantum effects theory of EOT, the transmitted energy spectral density $u[\mathrm{L}]\cdot[\mathrm{N}]\cdot[\mathrm{T}-1]$ of electromagnetic waves is determined by the Planck constant $h[\mathrm{L}]\cdot[\mathrm{N}]\cdot[\mathrm{T}]$, incident electromagnetic frequency $\omega[\mathrm{T}-1]$, incident electric field intensity $E[\mathrm{N}]\cdot[\mathrm{C}-1]$, dielectric constant $\varepsilon[\mathrm{L}-2]\cdot[\mathrm{N}-1]\cdot[\mathrm{T2}]$. Selecting aperture radius $r[\mathrm{L}]$ as the state variable, the parameters $m[\mathrm{L2}]$ and $n[\mathrm{L3}]$ can be expressed as follows:

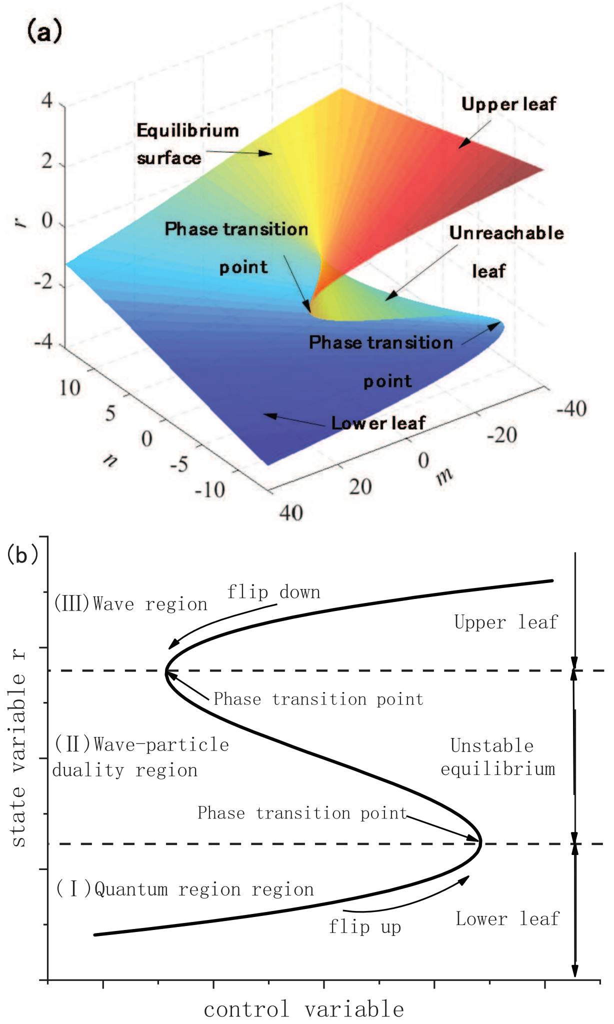

Fig. 1: (a) The equilibrium surface of standard cusp catastrophic model; (b) non-equilibrium phase transition path.

$$\begin{cases} m = Ah^{a}\omega^{a_1}E^{a_2}\varepsilon^{a_3}u^{a_4}, \\ n = Bh^{a}\omega^{a_1}E^{a_2}\varepsilon^{a_3}u^{a_4}, \end{cases} \tag{3}$$

where A and B are the constants, Planck constant h and frequency ω represent microscopic scale parameters, while electric field intensity E and dielectric constant ε represent macroscopic scale parameters. Table 1 shows the dimensions of physical variables. By the dimensionless analysis, the power exponents satisfy the following relationships, as

Table 1: Dimensional relationship of power exponent among parameters.

	$h(\alpha)$	$\omega(\alpha_1)$	$E(\alpha_2)$	$\varepsilon(\alpha_3)$	$u(\alpha_4)$
L	1	0	0	-2	1
N	1	0	1	-1	1
T	1	-1	0	0	-1
C	0	0	-1	2	0

shown in equation:

$$\begin{cases} a-2a_3+a_1=2, \\ a+a_2-a_3+a_4=0, \\ a-a_1-a_4=0, \\ -a_2+2a_3=0, \end{cases} \quad \begin{cases} a-2a_4+a_4=3, \\ a+a_3-a_4+a_4=0, \\ a-a_1-a_4=0, \\ -a_2+2a_3=0. \end{cases} \tag{4}$$

The following expressions for m and n are obtained:

$$\begin{cases} m = Ah^a\omega^{\frac{6a-2}{3}}E^{-\frac{4}{3}}\varepsilon^{-\frac{2}{3}}u^{\frac{2-3a}{3}}, \\ n = Bh^{\frac{3a+1}{3}}\omega^{\frac{6a-1}{3}}E^{-2}\varepsilon^{-1}u^{\frac{2-3a}{3}}. \end{cases} \tag{5}$$

The quantitative relationship of the transmitted energy spectral density $u(r,w,a)$ with aperture radius r, incident electromagnetic frequency ω, and index a can be expressed as

$$u\,(r,w,a) = \Big(-Ah^a\omega^{\frac{6a-2}{3}}E^{-\frac{4}{3}}\varepsilon^{-\frac{2}{3}}r^{-2} - Bh^{\frac{3a+1}{3}}\omega^{\frac{6a-1}{3}}E^{-2}\varepsilon^{-1}r^{-3}\Big)^{\frac{3}{3a-2}}. \tag{6}$$

As shown in fig. 2, the variation of transmitted energy spectral density u with aperture radius r and index a is presented under a certain incident electromagnetic frequency ω. We define the exponential term a as the quantum transition factor. When quantum transition factor $a = 0$, the physical quantity h at the microscale does not exist, the incident wave shows the volatility of light and passes through the aperture to produce a diffraction fringe. It is meaningful that when $a = 1/6$, there exists $\frac{-6}{3a-2} = 4$, which is in accordance with $(r/\lambda)^4$ law of Bethe's aperture theory. Thus, the transmitted energy spectral density is very low and only the diffraction light influence is present. While the quantum transition factor a increases gradually, the incident wave gradually reveals some of the particle properties, and the field edge effect gradually appears, which results in a profound field enhancement in the exit region and leads to the enhanced transmittance. The range $1/6 < a < 0.8$ is the wave-particle duality region, the incident wave shows both wave-particle duality, and the edge effect and diffraction phenomenon exist simultaneously. As the value of a continues to increase, the diffraction phenomenon decreases and the edge effect gradually increases, which leads to the increase of transmission. When $a = 0.87$, the transmitted energy spectral density has the maximum value, then the volatility of the incident light disappears, and the incident wave shows particle-like nature of light completely. The range $0.87 < a < 1.0$ is macroscopic quantum region, the transmitted energy spectral density decreases rapidly with the increase of a.

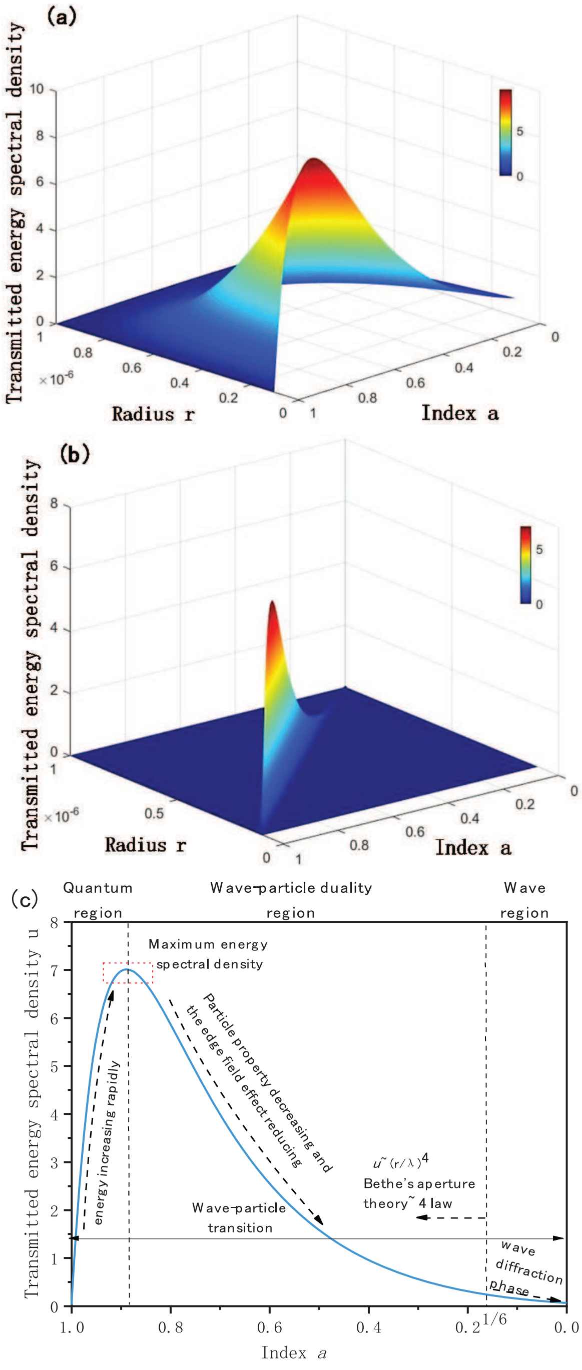

Fig. 2: (a) Relationship among transmitted energy spectral density u, index a and radius r; (b) the cross-sectional figure of transmitted energy spectral density u; (c) relationship between transmitted energy spectral density u and index a.

Verification of this analysis method. – According to thin microcavity theory, the dimensional parameters of the single subwavelength aperture include circular aperture of radius r, thickness of the microcavity h, and the incident E-polarized plane wave with wavenumber k_0 (where $k_0 = 2\pi/\lambda$) is used to illuminate the nanostructure along the z-axis, where $\Phi_i = E_0 \exp(ik_0 z)\, y$. The governing equation of the electromagnetic field distribution in a thin film with a uniform thickness under an external light incidence is derived. Then the magnetic field component H_3 in thin microcavity can be obtained as

$$H_3 = \sum_{n=0}^{\infty} \left[A_n J_n(kr) + C_n I_n(kr) + E_0 r^n \frac{3}{\pi h^2 i} \frac{{k_0}^2}{\omega \mu k^4} \times e^{ik_0 h/2} \frac{(-1)^{n+1} - 1}{(n+1)\, n! 2^{n+1}} \right] \exp(in\theta). \qquad (7)$$

In addition, the other electromagnetic field components can also be obtained. Therefore, we get the accurate distribution of electromagnetic field inside and outside of the thin microcavity under an incident plane wave. Based on eq. (7) and the relationship between the components of the electromagnetic field, the normalized transmission can be calculated as

$$u = \frac{\boldsymbol{P}_{out}}{\boldsymbol{P}_{in}} = \frac{\frac{1}{2}\int \varepsilon {\Phi_t}^2 \mathrm{d}s}{\frac{1}{2}\int \varepsilon {\Phi_i}^2 \mathrm{d}s}, \qquad (8)$$

where $\boldsymbol{P}_{\mathrm{out(in)}}$ is the power flux out of (in) the thin microcavity, $\Phi_{t(\mathrm{i})}$ is the electric field intensity out (in) the thin microcavity, and S is the area of the subwavelength aperture.

In order to verify the accuracy of the catastrophe model, the results are verified by comparison with those calculated by the thin microcavity theory. The specific parameter that is used for this analysis of the transmittance consists of the following components: the incident wavelength $\lambda = 630\,\mathrm{nm}$ in the visible spectrum, the corresponding critical radius $R_0 = 300\,\mathrm{nm}$. Thickness of the microcavity is selected to be 20 nm in this paper based on the assumption that the film thickness is much smaller than the incident wavelength.

Figure 3 shows the relationship between normalized transmission and thin microcavity radius r under the condition of constant incident wavelength $\lambda(\lambda = 630\,\mathrm{nm})$, where the transmittance based on thin microcavity theory and cusp catastrophe model are shown as the blue and red lines, respectively. According to the variation of aperture size of thin microcavity, the whole transition process can be divided into three stages: macroscopic quantum region wave-particle duality region and wave region, respectively. In macroscopic quantum region, the transmittance increases rapidly with the increase of the thin microcavity radius in the range of 10–150 nm ($\lambda/60$–$\lambda/4$), the incident wave shows more particle-like nature of light and excites the field edge effect. As the radius increases, the incident light flux increases, resulting in a rapid increase in transmittance and there is an enhanced transmission peak at the radius 150 nm ($\lambda/4$), where the transmittance is larger than 7. In wave-particle duality region, the transmittance begins to decrease rapidly with the increase of the thin microcavity radius in the range of 150–300 nm ($\lambda/4$–$\lambda/2$), the incident wave shows both wave-particle duality, and the edge effect and diffraction phenomenon exist simultaneously. As the radius increases, the field edge effect gradually decreases, resulting in a rapid decrease in transmittance. In wave region, the incident wave shows

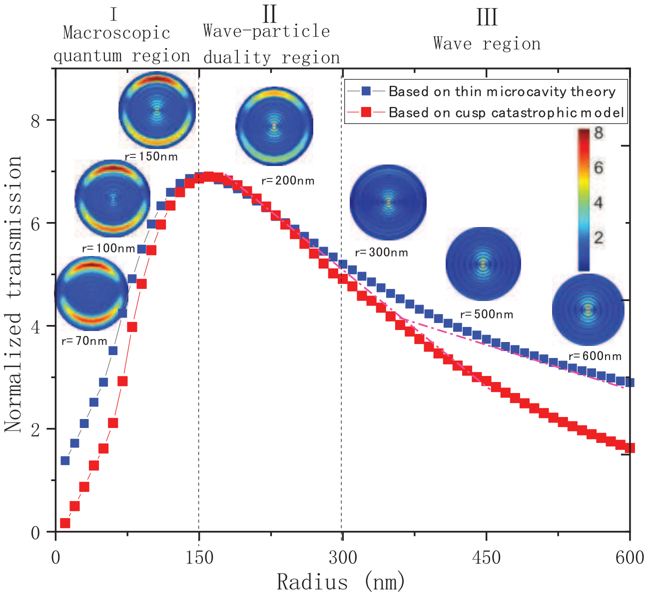

Fig. 3: The relationship between normalized transmission and thin microcavity radius r under the condition of constant incident wavelength λ, where $\lambda = 630\,\mathrm{nm}$.

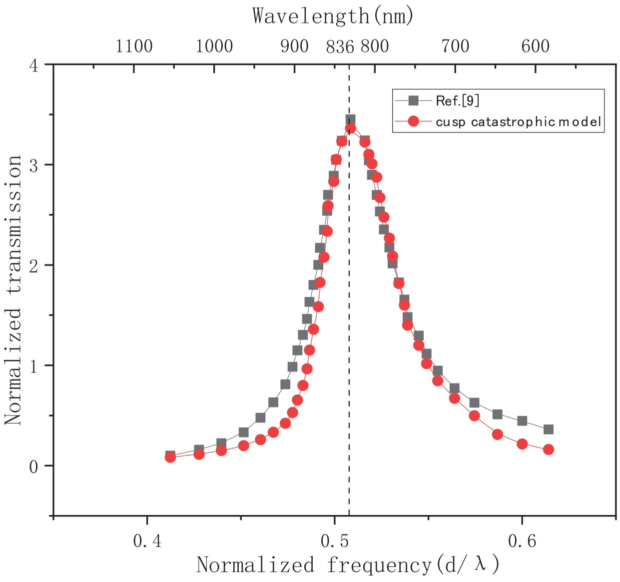

Fig. 4: The relationship between normalized transmission and incident wavelength of the thin microcavity. The up (down) horizontal axis is labeled as the wavelength (frequency), where $d = 425\,\mathrm{nm}$.

the volatility of light and passes through the aperture to produce a diffraction fringe. As the radius increases, the particle-like nature of the incident light disappears, the transmittance decreases slowly and tends to be flattened gradually in the range of 300–600 nm ($\lambda/2$–λ). In summary, the results calculated based on the catastrophic model agree well with the thin microcavity theory and the relative error is within 5%.

Figure 4 shows the relationship between normalized transmission and incident wavelength λ. The diameter of the thin microcavity d is fixed ($d = 425\,\text{nm}$) and incident wavelength ranges from 600 nm to 1100 nm, the EOT corresponds to the peaks in the transmission at the wavelength $\lambda = 836\,\text{nm}$ and the relationship between wavelength and diameter of the thin microcavity is $d/\lambda = 0.5$, which verifies the accuracy of the cusp catastrophe model.

Conclusions. – In this paper, a quantitative expression of transmitted energy spectral density about EOT is derived by the cusp catastrophe model, and the quantum transition factor is obtained to describe the whole wave-particle transition. Besides, Bethe's aperture theory is only one of our special cases in catastrophe model. The accuracy of catastrophe model is verified by comparing the thin microcavity theory and literature data, and the influence of incident frequency ω and thin microcavity radius r on the transmittance are analyzed. These results unveil a better understanding of the EOT, which can be used in various fields, such as light sensors and optical tweezers.

* * *

The authors declare no conflicts of interest.

Data availability statement: The data that support the findings of this study are available upon reasonable request from the authors.

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