Bloch states in light transport through a perforated metal

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Abstract – Light transport in a metal with two-dimensional hole arrays is considered. Analytical expressions for a transmission coefficient in periodic, isolated and disordered cases are derived, assuming the existence of waveguide modes transverse tunneling in a two-dimensional plane perpendicular to the traveling direction of light. The one-dimensional case of periodic holes, due to its simplicity, is investigated in detail. In the dilute metal regime, when metal fraction is small, our numerical study of the transmission coefficient of the central diffracted wave indicates the existence of a minimum which is completely independent of an incident wavelength. Further increasing of the metal fraction leads to the unusual monotonic increasing of the central-diffracted-wave transmission. The role of the surface plasmons is discussed.

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Introduction. – Since its discovery [1] the extraordinary optical transmittance (EOT) has attracted great interest. This interest is largely motivated by a recent progress in nanotechnology which allows to get for EOT a possible applications in different optical devices. Many experimental and theoretical papers have been devoted to the study of the EOT (for a review, see ref. [2]). The phenomenon of EOT seemed to be well understood [3,4] with the involving of the surface plasmons and Bloch states. The former appeared on the interface between metal and dielectric, while the Bloch states originated by the periodicity of hole arrays. So far, in theoretical understanding of EOT much attention was paid to the plasmon aspect of the problem [5,6] and less attention to the Bloch states and periodicity (see, e.g., ref. [7] and references therein). The Bloch states of plasmons on the periodically perforated metal surface were studied in ref. [8], taking into account the mechanism of plasmons’ vertical tunneling from one metal surface to another one. This parallel to the traveling direction of the light mechanism eventually converts coupled surface plasmons on the two surfaces of the film to free photon states that contribute to the EOT phenomenon. Another type of tunneling mechanism, in addition to the vertical tunneling, that can coexist in such systems, is the transverse tunneling on a two-dimensional surface, perpendicular to the traveling direction of light. The latter mechanism, due to the interference and diffraction of the surface waves excited by light incident on the perforated metal surface, may affect the electromagnetic waves transport and play an important role in causing large transmission (see, e.g. refs. [9–11]).

In the present paper, without pretending to present a complete mathematical description of the theory of EOT, we develop a different approach to study the behavior of electromagnetic waves in a periodically performed metal system taking into account the existence of waveguide modes transverse tunneling on a two-dimensional surface perpendicular to the traveling direction of light. We have concentrated our attention on the role of the Bloch states and show that this mechanism with a transverse waveguide modes tunneling leads to peculiarities in light transport. Particularly, in the dilute case when metal fraction is small, we have found an independence of the transmission coefficient of the central diffracted wave from the incident wavelength and its unusual increase with the increase of the metal fraction. We explicitly derived an analytical expression for the transmission coefficient in the disordered hole arrays case. We found that without Bloch states the disordered hole arrays lead to the broadening of the spectral shape in accordance with refs. [12,13].

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where $k$ plays the role of the time) and the time-dependent Schrödinger equation for a particle with mass $m$ is presented below.

\[ \nabla^2 \phi(x,y,z) + k_0^2 \varepsilon(x,y) \phi(x,y,z) = 0, \]  
(1)

where $k_0 = \omega/c$ is the wave number corresponding to the angular frequency $\omega$ of an incident photon and $\varepsilon(x,y)$ is the two-dimensional periodic dielectric permittivity of the system. Equation (1) is valid for $s$ and $p$-polarized waves and the scalar function $\Phi$ describes the transverse components of an electric or a magnetic fields, respectively.

Mainly following refs. [14–16], we seek the solution of the wave propagating in the system as a product of a fast and a slowly varying, $\phi(x,y,z)$, function on a wave incident $z$-direction, implying that the metal fraction of our system is small, 

\[ \Phi(x,y,z) = e^{ik_0z}\phi(x,y,z). \]  
(2)

Note that this situation differs from the most of EOT considerations where usually the opposite case is considered.

Substituting eq. (2) into eq. (1) and neglecting the second derivative of $\phi$ with respect to $z$ (\(|d^2\phi/dz^2| < 2k_0|d\phi/dz|\)), one gets

\[ i\frac{d\phi}{dz} = \hat{H}(x,y)\phi, \]  
(3)

where

\[ \hat{H}(x,y) = -\frac{1}{2k_0}\nabla^2 + \frac{k_0}{2}(1-\varepsilon(x,y)) \]  
(4)

and $\nabla^2 \equiv (\partial^2/\partial x^2 + \partial^2/\partial y^2)$. Note that despite the presence of a surface charge on an interface metal-dielectric, the parabolic approximation, that is $|d^2\phi/dz^2| < 2k_0|d\phi/dz|$ is justified. The reason is that the surface charge causes a discontinuity in the perpendicular component of the electric field. In the geometry (see fig. 1) discussed above, the electric field normal to the surface component is absent and the wave function in eq. (1) is the transverse component of the electric field that is continuous on the surface. The criterion of smallness of its second derivative is presented below.

The obvious similarity of eq. (3) (the spatial coordinate $z$ plays the role of the time) and the time-dependent Schrödinger equation for a particle with mass $m_0$, moving in the two-dimensional potential $V(x,y) = k_0^2 (1-\varepsilon(x,y))$ may be used as a starting point to evaluate the wave transmission coefficient at $z$.

The solution of eq. (3) can be represented through the eigenfunctions of the Hamiltonian equation (4),

\[ \phi(x,y,z) = \sum_n c_n e^{-iE_n z}\phi_n(x,y) \]  
(5)

and

\[ \hat{H}\phi_n(x,y) = E_n \phi_n(x,y). \]  
(6)

Finally, the substitution of eq. (5) into eq. (2) yields the solution of the Maxwell equation

\[ \Phi(x,y,z) = e^{ik_0z}\sum_n c_n e^{-iE_n z}\phi_n(x,y). \]  
(7)

It follows from eq. (7) that the local transmission amplitude of a central diffracted wave can be defined as

\[ t(x,y) = \sum_{E_n < k_0} c_n e^{-iE_n L}\phi_n(x,y), \]  
(8)

where $L$ is the system size in the $z$-direction.

Before entering into a more detailed analysis of the local transmission amplitude, let us note that if we ignore the losses and take into account that the metal dielectric constant in the optical region is a real large negative number, then i) the potential energy term $V(x,y) = k_0^2 (1-\varepsilon(x,y))$ in the Hamiltonian equation (4) is positive everywhere; ii) correspondingly, all $E_n$ are also real and non-negative $E_n \geq 0$ and iii) exploiting $|d^2\phi/dz^2| < 2k_0|d\phi/dz|$ leads to the condition $E_n < 2k_0$.

The central-diffracted-wave transmission coefficient that is measured in the experiment can be estimated by using the following expression:

\[ T = \frac{1}{S} \int dx dy |t(x,y)|^2, \]  
(9)

where $S$ is the area of the system. Substituting eq. (8) into eq. (9), one has

\[ T = \frac{1}{S} \sum_{E_n < k_0} |c_n|^2. \]  
(10)

In order to find the coefficients $c_n$, let us consider eq. (7) for $z = 0$,

\[ \Phi(x,y,z = 0) = \sum_n c_n\phi_n(x,y). \]  
(11)

Next, we assume that the wave impinging to the system has an amplitude 1 (the region $z < 0$). From the continuity at $z = 0$, one has $\Phi(x,y,z = 0) = 1 + r(x,y)$, where $r(x,y)$ is a local reflection coefficient which for the metal without holes is approximately $-1$. Clearly, the existence of the holes will change the value of $r$. However, this change will not affect the further calculations, and for
this reason in our further calculations, for the reflection coefficient we assumed some average value \( r \) close to zero provided that the metallic fraction is small. Within this approach, multiplying both sides of eq. (11) by \( \phi_n^*(x, y) \) and integrating over the surface, one has
\[
c_n = (1 + r) \int dx dy \phi_n^*(x, y). \quad (12)
\]
Substituting eq. (12) into eq. (10), we arrive at the final result for the transmission coefficient
\[
T = \frac{|1 + r|^2}{S} \int_{E_n < k_0} d\vec{p} d\vec{p}' \phi_n^*(\vec{p}) \phi_n(\vec{p}'), \quad (13)
\]
where \( \vec{p} \equiv (x, y) \) is a two-dimensional vector on the \( xy \) plane.

This is our main general result. In the following sections we analyze its limits for different models.

To close this section let us note that if the dielectric permittivity \( \varepsilon(x, y) \) is a periodical function, then the spectrum of the Hamiltonian equation (4) consists of allowed and forbidden energy bands. As for the transmission coefficient, it depends on the position of the incident wave number in the transverse energy spectrum.

**Bloch states.** As follows from eq. (13), the transmission coefficient equals zero provided that \( k_0 < E_b \), where \( E_b \) is the bottom value of the first energy band. When \( k_0 \) lies in the zone, using the Bloch states the transmission coefficient can be rewritten in terms of a quasi-momentum \( \vec{q} \) as
\[
T = \frac{|1 + r|^2}{2} I, \quad (14)
\]
where
\[
I = \frac{1}{S} \int_{E(\vec{q}) < k_0} \frac{dq}{2\pi} \int d\vec{p} d\vec{p}' \phi_n^*(\vec{p}) \phi_n(\vec{p}'). \quad (15)
\]
Here the integration over the quasi-momentum \( \vec{q} \) is carried out over the first Brillouin zone \( -\pi/a \leq q_x \leq \pi/a, -\pi/b \leq q_y \leq \pi/b \) and \( a, b \) are periods of \( \varepsilon(x, y) \) in the \( x \) and \( y \) directions, respectively. According to the Bloch theorem the eigenstate \( \phi_q \) in a periodical potential can be represented in the form
\[
\phi_q(\vec{p}) = e^{i\vec{q}\cdot\vec{p}} u_q(\vec{p}), \quad (16)
\]
where \( u_q(\vec{p}) \) is a periodical function satisfying the equation
\[
\left[ -\frac{1}{2k_0}(i\vec{q} + \vec{V}(\vec{p}))^2 + V(\vec{p}) \right] u_q(\vec{p}) = E(\vec{q}) u_q(\vec{p}). \quad (17)
\]
For simplicity and as an illustration of the approach, we will carry out a further consideration in the one-dimensional case. We hope that the results, obtained in this particular case will enable us to understand, at least at the qualitative level, the transmission of an electromagnetic wave in a three-dimensional system in the presence of a transverse waveguide modes tunneling.

**Kronig-Penney model.** Suppose that slits are periodicaly placed on the \( x \)-axis, which is transverse to the direction of propagation. A cross-section of the potential in the \( x \)-direction can be presented as an array of square potential wells. A metal part will serve as a barrier and characterized by width \( b \) and period \( a \). A width of a slit is \( a - b \), correspondingly. The metallic dielectric constant described by the Drude model \( \varepsilon_m = 1 - \omega_p^2/\omega^2 \) and the height of a barrier is defined as \( V_m = k_p^2/2k_0 \) (\( k_p = \omega_p/c \) and \( \omega_p \) is the plasma frequency of a metal). The vacuum part dielectric is described by \( \varepsilon = 1 \) and with a potential energy \( V = 0 \). For a metal in the optical region usually \( V_m > k_0 \). Because only the energies \( E_n < k_0 \) give a contribution to the transmission coefficient \( T \), we will consider the case \( E < V_m \) when finding the spectrum of the Hamiltonian equation (4). The quantum-mechanical problem, eq. (4), is reduced to the well-known Kronig-Penney model [17]. Let us write \( I \), defined by eq. (15), for the one-dimensional case,
\[
I = \frac{1}{L} \int_{E(\vec{q}) < k_0} \frac{dq}{2\pi} \int dx dz \phi_q(x) \phi_q(x'). \quad (18)
\]
Using the Bloch theorem \( \phi_q(x) = e^{iqx} u_q(x) \), with \( u_q(x) \)-periodical function, one obtains
\[
I = \frac{1}{L} \int_{E(\vec{q}) < k_0} \frac{dq}{2\pi} \sum_{nm} e^{iqa} dxe^{-iqz} u_q(x) \times \int_{(m-1)a}^{ma} dx e^{iax} u_q(x). \quad (19)
\]
Changing the variables one finds
\[
I = \frac{1}{L} \int_{E(\vec{q}) < k_0} \frac{dq}{2\pi} \sum_{n} e^{-iqa} \times \int_{0}^{a} dx e^{iax} u_q(x), \quad (20)
\]
where the wave function in the unit cell and in the different regions is found from eq. (17),
\[
u_{q1}(x) = (A \cos \beta x + B \sin \beta x) e^{-iqx}, \quad 0 < x < a - b, \quad (a)
\]
\[
u_{q2}(x) = (A \cosh \alpha x + D \sinh \alpha x) e^{-iqx}, \quad a - b < x < a \quad (b)
\]
with \( \beta = \sqrt{2k_0E} \) and \( \alpha = \sqrt{2k_0(V_m - E)} \).

Substituting \( \sum_n e^{-ina} = 2\pi \delta(qa) \) into eq. (21), one obtains
\[
I = \frac{1}{a} \left[ \int_{0}^{a} u(x) dx \right]^2, \quad (22)
\]
where \( u(x) \equiv u_{q=0}(x) \) is determined by eq. (21). The constants \( B, C, D \) can be expressed by \( A \) using boundary conditions. A itself can be found from the normalization condition \( \int_{0}^{a} |u(x)|^2 dx = 1/N \), where \( N = L_x/a \) is the number of unit cells. Using the continuity at \( x = 0 \), one gets \( C = A \). From the continuity of \( du/dx \) at \( x = 0 \), one has \( B\beta = Da \). Finally from the continuity of \( u(x) \) and
du/dx at \( x = a - b \) and periodicity \( du_1(x)/dx|_{x=a-b} = du_2/dx|_{x=a-b} \), one has
\[
A [\cos \beta(a - b) - \cosh ab] + B [\sin \beta(a - b) + \beta/a \sinh ab] = 0,
\]
\[
A [\alpha \sinh ab - \beta \sin(\beta(a - b))] + B [\beta \cos \beta(a - b) - \beta \cosh ab] = 0.
\]
(23)

Equalizing the determinant of a 2 × 2 homogeneous equation to 0 one gets the dispersion relation for \( q \):
\[
1 = \frac{a^2 - \beta^2}{2a} \sinh ab \sin(\beta(a - b)) + \cosh ab \cos(\beta(a - b)).
\]
(24)

Expressing now coefficient \( B \) through \( A \) according to eq. (23) and taking elementary integrals we finally arrive at the expression for \( I \):
\[
I = \frac{8}{\alpha \beta a} \left[ \frac{\alpha \tan \left( \frac{\beta(a - b)}{2} \right) + \beta \tanh \left( \frac{ab}{2} \right) \cosh \alpha a}{2} \right]^2
\]
\[
\times \left[ 2 \alpha \tan \left( \frac{\beta(a - b)}{2} \right) + 2 \beta \tanh \left( \frac{ab}{2} \right) \cosh 2\alpha a \right]
\]
\[
+ \alpha \alpha^2 \beta + \alpha \beta \tan^2 \left( \frac{\beta(a - b)}{2} \right) \left( a - b - \beta^2 \alpha \beta \right)^{1/2} \right]^{-1}.
\]
(25)

Note that the above expression has been derived using the first relation of eqs. (23). However, using the dispersion relation (24), one can easily show that the second relation leads the same result. In fig. 2 we present the function \( I \) vs. \( b/a \) for \( k_p = 4.6 \times 10^{-2} \text{ nm}^{-1} \) (silver Ag) and \( k_p = 1.84 \times 10^{-2} \text{ nm}^{-1} \) (potassium K) (in both cases the wave number of an incident photon is \( k_0 = 10^{-2} \text{ nm}^{-1} \)). We have checked that the presented curves are unaffected by the change of \( k_0 \) in the visible region \( 0.62 \times 10^{-2} < k_0 < 1.57 \times 10^{-2} \text{ nm}^{-1} \). This means that for a given period \( a \) and \( k_p \), all the curves can be scaled into a single curve. The physical reason of the \( k_0 \) independent of the results is in the structure of the dispersion relation (24). The latter, in the frame of the adopted approach, can be described by a mean of the unique combination \( k_0 \).

Fig. 2: Plot of the function \( I(b/a) \) on a metal fraction for two values of \( k_p \) (silver and potassium). The wave number of an incident photon is \( k_0 = 10^{-2} \text{ nm}^{-1} \).

Relatively small metal barrier height and with large tunneling rate across a barrier, the central-diffracted-wave transmission coefficient (square symbol) increases with the further increase of the metal fraction (see fig. 2). This leads to some focusing effect in a central diffraction direction.

Note that the transmission coefficient \( T \), eq. (14), includes also the multiplier \( |1 + r|^2 \) which, in contrast to \( I \), decreases with increasing \( b/a \). However, the rate of the decrease of \( |1 + r|^2 \) is much slower than the rate of the increase of \( I \), and, as a result, the central-diffracted-wave transmission coefficient is increasing with \( b/a \). Such an unusual behavior is caused by periodicity and Bloch states. It is easy to get convinced that in the case of isolated slits, where the wave functions overlap is negligible and where Bloch states cannot exist, \( T \) behaves totally differently.

**Isolated slits.** – For large plasmonic wave number \( k_p \), the band width becomes very narrow. The reason for this is that \( k_p \) determines the barriers height and large \( k_p \) suppresses tunneling through the barrier. In this case the transversal wave functions become less and less extended in space and more localized within a hole with negligible overlap. In this limiting case one can use the infinite potential well approximation to evaluate the transmission coefficient (13). Writing the wave functions in the form [18]
\[
\phi_n(x) = \sqrt{\frac{2}{a-b}} \sin \frac{n\pi x}{a-b}
\]
and substituting eq. (26) into eq. (13), we find
\[
T_{is} = \frac{8|1 + r|^2 a - b}{\pi^2 a}. \tag{27}
\]

We arrived at the above expression summing over all the independent slit contributions and restricted ourselves by terms \( n = 1 \) while calculating the sum in eq. (13). The contributions of terms with \( n > 1 \) become irrelevant because \( k_0 < E_0 \) and, therefore, only the first band gives a contribution to the transmission.

Comparing eq. (27) with the maximal value, one has \( T_{is}/T_{max} \sim \frac{a-b}{a} \). As expected, for isolated holes the
transmission coefficient becomes size dependent, that is $T_{1s}/T_{\text{max}}$ is proportional to the fraction of the vacuum part in the system. In this sense, the isolated holes system reveals a usual dependence of the transmission coefficient on the metal fraction. We expect to find the same ratio to be valid also in the case of a two-dimensional hole array.

**Disordered hole arrays.** – In this case it is convenient to represent the transmission coefficient, eq. (13), in the form

$$ T = \frac{1 + r^2}{S} \int_{0}^{k_0} dE \left( \sum_n \delta(E - E_n) |\phi_n(0)|^2 \right), $$

(28)

where $\langle \ldots \rangle$ means averaging over the random positions of holes and $\phi_n(\vec{r})$ is the Fourier transform of $\phi_n(\vec{r})$ satisfying the Schrödinger equation with random potential

$$ \left[ -\frac{1}{2k_0} \nabla^2 + V(\vec{r}) \right] \phi_n(\vec{r}) = E_n \phi_n(\vec{r}), $$

(29)

where $V(\vec{r})$ is assumed to be a Gaussian distributed random function with a correlator $B$, $B = \frac{1}{2} \int d\vec{r} V(\vec{r})^2 = k_0 (1 - \epsilon_m) (1 - f_v)/2$ and $f_v$ is the fraction of the vacuum part (in the 1D periodic system, as discussed in the previous section $1 - f_v = b/a$).

We now turn to the calculation of the transmission coefficient, eq. (28). In order to carry out averaging over the randomness, it is convenient to express the latter quantity through the average Green’s function,

$$ T = \frac{1 + r^2}{S} \int_{0}^{k_0} dE \frac{1}{\pi} \langle -\text{Im} G_E(q = 0) \rangle $$

(31)

with $G_E = [E - H + i\delta]^{-1}$.

The averaged Green’s function can be represented in the form [19]

$$ (G_E(q)) = \frac{1}{E + V - \Sigma}, $$

(32)

where $\Sigma = \sum_{n \geq 2} \Sigma_n$ is the self-energy constituting contributions of irreducible parts of different order. Furthermore, we will restrict ourselves to the first term in the sum,

$$ \Sigma_2(q) = \int \frac{dk}{(2\pi)^2} B(|\vec{q} - \vec{k}|) G_0(k), $$

(33)

where $G_0(q) = [E - q^2/2k_0 + i\delta]^{-1}$ is the bare Green’s function.

The explicit form of correlation function $B(q)$ is needed to obtain a closed analytical expression for $T$, eq. (31). Particularly, in the limit of very small size $h \to 0$ holes, $B(q)$ can be substituted by $B(q = 0) = B_0 \sim f_v k_0^2 B_0 (1 - \epsilon_m)^2$. Evaluating the integrals in eqs. (31) and (33) we find

$$ T_d = \frac{|1 + r|^2}{\pi} \left[ \text{arctan} \frac{2(k_0 + V)}{k_0 B_0} - \text{arctan} \frac{2V}{k_0 B_0} \right]. $$

(34)

When obtaining eq. (34) we neglect Re$\Sigma$ relative to $V$. Expanding arctan functions in the limit $B_0 \to 0$, for the transmission coefficient in the disordered case, we finally obtain

$$ T_d = \frac{|1 + r|^2}{2\pi} \frac{k_0^2 B_0}{|\vec{k}_0 + \vec{V}|}. $$

(35)

The comparison of eqs. (27) and (35) shows important differences between the two cases, in spite of the formal factor $|1 + r(\omega)|^2$ (see ref. [13]). In the disordered case, eq. (35), contrary to the periodic case, $r(\omega)$ has no peculiarities and is a smooth function of $\omega$. This means that the randomness destroys the resonant spectral shape and leads to its broadening [12,13], assuming that the second multiplier in eq. (35) is a smoothly varying function of the frequency. This is true for almost all accepted metallic models and can be seen using the explicit form of the dielectric constant $1 - \epsilon_m = \omega_p^2/\omega^2$, $B_0$ and $V$.

By comparing with the isolated case contribution, eq. (27), and assuming that $\nabla \sim k_0$ and $B_0 \to 0$, one finds

$$ T_d \sim k_0^2 h^2. $$

(36)

It follows from eq. (36) that in the disordered case the transmission coefficient $T_d$ much smaller than $T_{1s}$ provided that $k_0 h \ll 1$. Two coefficients become of the same order when $k_0 h \sim 1$.

**Conclusion and discussion.** – We have discussed the problem of light transport through a perforated metal, taking into account the transverse waveguide modes tunneling in a two-dimensional plane perpendicular to the traveling direction of light. Periodic, isolated and disordered holes systems are analyzed in detail. Analytical expressions are derived for all different regimes. The onedimensional case of periodic holes, due to its simplicity, is investigated in detail. In the dilute metal regime, when the metal fraction is small, our numerical study of the transmission coefficient of the central diffracted wave indicates the existence of a minimum which is completely independent of an incident wavelength. The transmission coefficient of the central diffracted wave increases when the metal fraction of the system is increasing. The main contribution to the transmission coefficient is connected with extended states that are close to the center $q = 0$ of the Brillouin zone. This means that in order to observe the above-mentioned peculiarities in perforated systems, it is enough that the system exhibits long-range or quasi-long-range structural order in the $xoy$ plane (see also ref. [20]).

In our discussion we take into account the influence of a transverse tunneling between different holes on the transmission coefficient $T$. As a result, $T$ does not depend on the system thickness in the $z$-direction (we ignore the imaginary part of $\epsilon$). Obviously, the exponential decaying of $T$ with thickness will arise if one takes into account the losses.

In our consideration we substitute a local reflection coefficient by an average value. This assumption seems more
relevant in the random hole arrays case. However, even in the periodical case one can imagine \( r(\omega) \) as a quantity that correctly takes into account periodical hole arrays similar to periodical gratings [21]. Note that all plasmonic effects are included into \( r(\omega) \). Particularly on impinging of \( p \)-polarized light a plasmon is generated on the perforated surface. The reflection coefficient close to the plasmonic resonance becomes minimal [21] leading to the maximal value of the transmission coefficient. Plasmonic resonance takes place when the plasmon wave number coincides with one of the photonic crystal reciprocal lattice periods, see, for example, [22]. Note that \( r(\omega) \) depends on the geometry of the perforated surface and can detect resonance effects associated with the geometry of holes [23].

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