Graded transmission in a bent orifice

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We calculate the transmission of a bent orifice. The bending angle φ is assumed to be small [$\varphi \ll 1$ and also $\theta \equiv \sqrt{(\omega-\omega_c)/\omega_c} \ll 1$, where ω is the incoming particle energy, and $\omega_c \equiv (\hbar\pi/L)^2/2m$ is the threshold one, L is the orifice width]. We find graded transmission: There is a critical angle $\varphi_c \approx \theta$. For $\varphi < \varphi_c$ $|t|^2 \cong 1$, and for $\varphi > \varphi_c$ the transmission is dropped abruptly to $|t|^2 \approx \theta^2$. We suggest an explanation for this phenomenon. [S0163-1829(99)01443-5]

A diffusive current is hardly affected by the lead topology. Hence, Ohm's law, which according to Einstein has a diffusive origin,[1] is the corner stone in any electronic devising. The engineers can layout very complicated circuits without being worried about the local curvature of a specific wire.

When quantum mechanics, and in more general any wave dynamics, is concerned the geometry of the wires boundaries cannot be ignored. The modifications of the boundaries geometry may cause wave scattering, diffraction and resonances and thus have an immense influence on the conductivity.

In the last two decades, when nanostructures fabrication became possible, the investigation of boundary effects turned out to be of practical importance. Many experimental (e.g., Refs. 2–7) and theoretical works (e.g., Refs. 8–13) were done on this field. In these references, one can see a huge diversity: abrupt changes in an orifice dimensions and quantum dots (e.g., Refs. 8–10), mesoscopical junctions (e.g., Refs. 3, 4, and 11), two-dimensional resonant tunneling structures (e.g., Ref. 6), rings of varying width (Ref. 13) etc.

In this paper, we investigate a very simple system: We calculate the transmission of a bent orifice (its width L and a bending angle φ). Although we choose a very small bending angle, the point of the twist is highly singular (see Fig. 1). We show that despite its simplicity, this system exhibits a peculiar and an unexpected behavior:

Let us define the parameter $\theta \equiv \sqrt{(\omega-\omega_c)/\omega_c}$ (where ω is the incoming energy and $\omega_c \equiv (\hbar\pi/L)^2/2m$ is the threshold one), then if $\theta > \varphi$ the scattered particle is hardly affected by the bend and the transmission is excellent, i.e., $|t|^2 \cong 1$, however when $\theta < \varphi$ the transmission dropped abruptly to $|t|^2 \approx \theta^2$ and remains at that value at least until $\varphi \approx 2\theta$. We give an explanation for this radical transmission change and for the emergence of the plateau. We also discuss the case of multiple-boundaries defects.

Let us consider the transmission of a thin but tilted orifice (Fig. 1). For simplicity, its width will be normalized to 1 (i.e., it is measured with the units of L). The stationary-state Schrödinger equation reads

$$\nabla^2 \psi(\mathbf{r}) + [\omega - V(\mathbf{r})]\psi(\mathbf{r}) = 0.$$

(Hereinafter we use the units $\hbar = 2m = 1$). V is the potential of the orifice walls ($V=0$ inside the orifice and $V=\infty$ on the outside) and ω is the energy of a *single* incident particle.

The incoming wave from the left ($x=-\infty$) is

$$\psi_{\rm inc} = \sum_n \sin k_n y (a_n e^{i\tilde{k}_n x} + r_n e^{-i\tilde{k}_n x})$$

while the transmitted one is

$$\psi_{\rm tran} = \sum_n \sin k_n y' (t_n e^{i\tilde{k}_n x'}).$$

Where a_n, r_n, and t_n are the incident, reflected, and transmitted coefficients, respectively,

$$k_n \equiv n\pi \quad \text{and} \quad \tilde{k}_n \equiv \sqrt{\omega - (n\pi)^2}.$$

The strategy is the following: $\psi_{\rm inc}$ is a solution in the entire ''left region.'' We do not say *yet* that this is the right one, but this is definitely a solution, because it solves the Schrödinger equation in all the ''left region,'' and it agrees with the boundary conditions of this region (except, for the moment, the one at $x=0$). The same thing goes for $\psi_{\rm trans}$; it solves the Schrödinger equation and maintains the boundary conditions in the entire ''right region.'' Therefore, it is a solution in this entire region.

Now, we need to find the right coefficients (a_n, r_n, and t_n), which will take care of the boundary condition at $x=0$, i.e., the continuity of the wave function and its derivative at $x=0$. In order to do so, we match the wave function and its derivative at N different points on the boundary $x=0$, then we take $N \to \infty$ and show that the solution (and the coefficients) converges to a specific function.

Let us define a new set of coordinates:

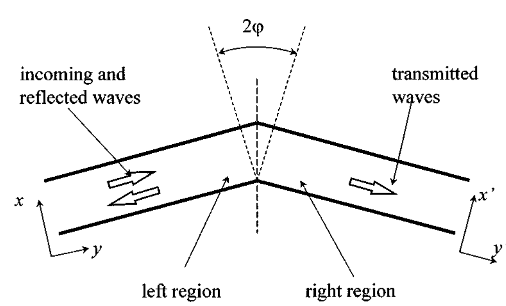

FIG. 1. An illustration of the bent orifice.

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

or equivalently

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} x' \\ y' \end{pmatrix}. \tag{1}$$

Then the wave function in the left side of the bend is

$$\sum_n \sin k_n(\xi \sin\varphi + \eta\cos\varphi)[a_n e^{i\tilde{k}_n(\xi\cos\varphi - \eta\sin\varphi)} + r_n e^{-i\tilde{k}_n(\xi\cos\varphi-\eta\sin\varphi)}], \tag{2}$$

and in the right one

$$\sum_n \sin k_n(-\xi\sin\varphi + \eta\cos\varphi)[t_n e^{i\tilde{k}_n(\xi\cos\varphi+\eta\sin\varphi)}].$$

With these notations, the matching of the wave function should take place at $\xi=0$. Limiting the calculations to N modes, the gluing of the wave function and its derivative at $\xi=0$ leads to 2 equations with $2N$ variables. In order to solve them, we quantize η

$$\eta^m \equiv \frac{m}{N\cos\varphi}, \quad 1 \leqslant m \leqslant N$$

(these are the N points were the matching takes place). The prescribed substitution solves this problem ($2N$ equations). The solution is straightforward

$$\mathbf{t} = \tau\cdot\mathbf{a}, \tag{3}$$

where $\mathbf{a}$ is the incident vector with the components a_n and $\mathbf{t}$ is the transmitted vector with the components t_n. τ is the transmission matrix

$$\tau \equiv \tfrac{1}{2}(T^{-1}T^* - \tilde{T}^{-1}\tilde{T}^*), \tag{4}$$

where the components of the different T's are

$$T_m^n \equiv \sin(k_n\eta^m\cos\varphi)\exp(i\tilde{k}_n\eta^m\sin\varphi)$$

$$\tilde{T}_m^n \equiv [-k_n\sin\varphi\cos(k_n\eta^m\cos\varphi) + i\tilde{k}_n\cos\varphi\sin(k_n\eta^m\cos\varphi)]\exp(i\tilde{k}_n\eta^m\sin\varphi).$$

We restrict the discussion to very small bending angles and to very small incoming momentums, that is

$$\varphi \ll 1, \quad \omega-\pi^2 \ll 1.$$

It is obvious, that in this case, only the first mode is propagating, and thus it is the only mode that carries energy to infinity.

Before going on, let us define an incident angle

$$\theta \equiv \tan^{-1}(\sqrt{\omega-\pi^2}/\pi) \approx \sqrt{\omega-\pi^2}/\pi.$$

This angle has a simple meaning. If k_y and k_x are the incoming wave numbers, then

$$\theta = \tan^{-1}(k_x/k_y).$$

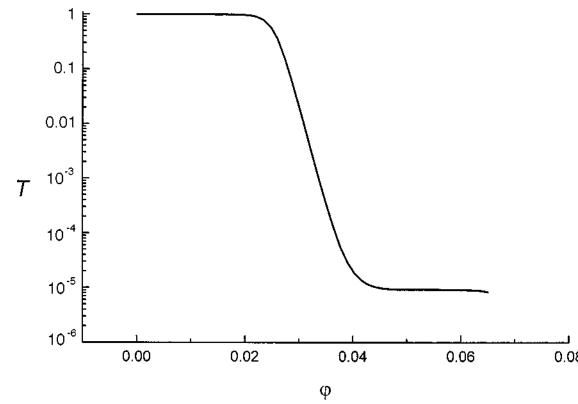

FIG. 2. The transmission ($T=|t|^2$) of the orifice as a function of the bending angle φ for $\omega-\pi^2=10^{-4}$ and $N=100$.

The plot in Fig. 2 was calculated for $\omega-\pi^2=10^{-4}$, i.e., $\theta \approx 3\times10^{-3}$, and $N=100$. From the graph we learn the following things: (a) For small angles, the transmission remains unity, i.e., $|t|^2=1$, in this regime it is actually a constant. (b) When φ exceeds a certain value $\phi_c \approx 0.025$ the transmission abruptly falls exponentially. (c) When φ exceeds the value ≈ 0.04 the transmission approaches a new plateau. This plateau lasts at least until $\varphi \approx 0.07$. (d) The value of the transmission in the second plateau is $\approx 10^{-5}$.

In order to see if these are true findings and not an artifact, we check them for different N's. Figure 3 presents the dependence of ϕ_c on N. As can be seen by the solid line it has an excellent fit with

$$\phi_c = \frac{p_1+p_2N}{p_3+N}, \tag{5}$$

where $p_2=(2.7\pm0.6)\times10^{-3}$. This p_2 is the extrapolated value of ϕ_c for $N\to\infty$. Hence, p_2 seems to be the ''real'' critical value φ_c. We can also see, that this value is very close to θ, i.e., $\varphi_c \approx \theta$. This is not by chance, it happens for every small θ. We will try to explain it later.

Next, we find that the plateaus values are independent of N. That is, for any number of modes the first plateau has the value 1, while the second one has the value $|t|^2 \approx \theta^2$.

We thus can summarize the results in the following expression:

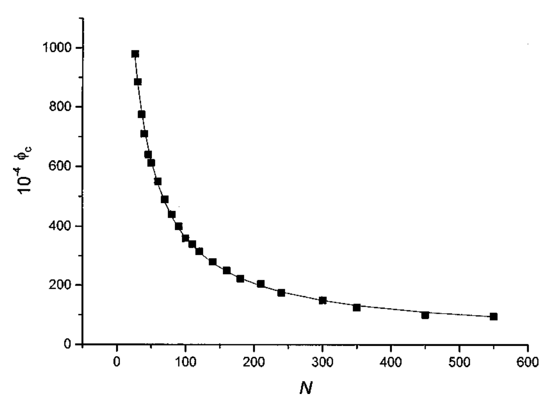

FIG. 3. The dependence of the transition angle ϕ_c on the matrix size (N). The solid line presents the fit $\phi_c=(p_1+p_2N)/(p_3+N)$ with $p_2=(2.7\pm0.6)\times10^{-3}$.

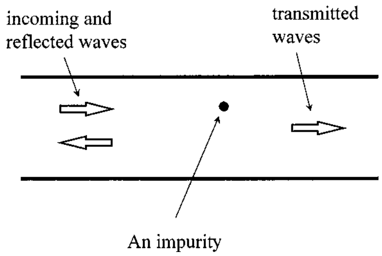

FIG. 4. 2D waves are scattered from a 2D point impurity within a thin orifice.

$$|t(\varphi)|^2 \approx \begin{cases} 1 & \varphi < \varphi_c \\ \theta^2 & \varphi > \varphi_c \end{cases}, \tag{6}$$

while $\varphi_c \approx \theta$.

Classically, there is a good explanation for $\varphi_c \approx \theta$, and for the plateau where $\varphi < \varphi_c$. One can easily be convinced, that classically for $\varphi < \theta/3$ all the particles are transmitted, while for $\varphi > \theta/3$ some of them are reflected, and the transmission decreases *linearly*. However, this description neither explains the critical nature of the change, nor does it give any reason for the second plateau (not to speak about its height).

A quantum mechanical explanation should be able to elucidate three points: (1.) Why for large bending angles (φ) does the transmission get the value $|t|^2 \to \theta^2$? (2.) Why does the transition take place at $\varphi \approx \theta$? (3.) And finally, why is there a plateau?

In order to face the first problem we consider the bent as a two-dimensional (2D) point defect. Thus, by doing so, we reduce the system to a scattering problem over a 2D impurity (see Fig. 4). Let us choose the 2D impurity potential function to be an impurity D function (IDF, see Ref. 14)

$$D(r) \approx W\delta(x)\exp[-(y-\varepsilon)^2/\rho^2], \tag{7}$$

where ρ is a characteristic width of the impurity and is assumed to be the smallest parameter of the problem, ϵ is the distance between the impurity and the lower boundary, W is a weight function, and $\delta(x)$ is the 1D Dirac's delta function. Then, the scattered function takes the form[16]

$$\psi_{\mathrm{scat}}(\mathbf{r}) = \psi_{\mathrm{inc}}(\mathbf{r}) - \frac{G(\mathbf{r},\mathbf{r}_0)\psi_{\mathrm{inc}}(\mathbf{r}_0)}{1+\int d\mathbf{r}' G(\mathbf{r}',\mathbf{r}_0)D(\mathbf{r}'-\mathbf{r}_0)} \times \int d\mathbf{r}' D(\mathbf{r}'-\mathbf{r}_0), \tag{8}$$

where $\mathbf{r}_0 \equiv \hat{y}\varepsilon$ is the place of the impurity, $\psi_{\mathrm{inc}}(\mathbf{r})$ is the wave function when the impurity is absent, and

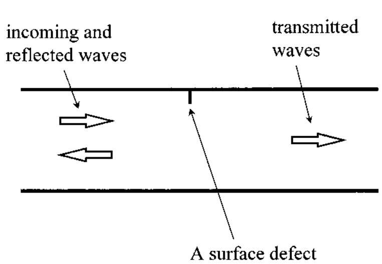

FIG. 5. The same as Fig. 4 but with a surface defect.

$$G(\mathbf{r},\mathbf{r}') \equiv \int \frac{dk}{2\pi} \sum_n \frac{\sin(n\pi y)\sin(n\pi y')}{E-(n\pi)^2-k^2} e^{ik(x-x')}, \tag{9}$$

is the 2D scattering Green function of our geometry. A more convenient way to write the Green function is

$$G(r,r') \equiv \sum_n \frac{\sin(n\pi y)\sin(n\pi\varepsilon)}{2i\sqrt{E-(n\pi)^2}} e^{i\sqrt{E-(nx)^2}|x-x'|}. \tag{10}$$

Then,

$$\int d\mathbf{r}' G(\mathbf{r}',\mathbf{r}_0)D(\mathbf{r}'-\mathbf{r}_0) = W\frac{\rho\sqrt{\pi}}{2i}\sum_n \frac{\sin^2(n\pi\varepsilon)}{\sqrt{E-(n\pi)^2}} e^{-(nx\rho/2)^2}. \tag{11}$$

Since we are interested in the regime of low energies, i.e., $E \approx \pi^2$, Eq. (11) can be approximated, except for the first term, to an integral

$$\approx W\frac{\rho\sqrt{\pi}}{2i}\left[\frac{\sin^2(\pi\varepsilon)}{\sqrt{E-\pi^2}} + \int_{\pi\rho}^{\infty}\frac{dy}{i\pi y}e^{-y/2}\sin^2(\varepsilon y/\rho)\right]. \tag{12}$$

Now we can investigate the case $\epsilon/\rho \gg 1$. This is the case where the impurity doesn't touch the boundary. In this case, the integral in Eq. (12) can be approximated to (in the limit $\rho \to 0$)

$$\frac{i}{4\pi}\{\ln[-(\pi\rho/2)^2]+\gamma\}. \tag{13}$$

A suitable choice for W in that case would be

$$W^{-1} = \frac{\rho}{4\sqrt{\pi}}\ln\left(\frac{\rho_b}{\rho}\right), \tag{14}$$

where ρ_b is some constant which is related to the De-Broglie's wavelength of the bound state of the impurity.

Then, we find that the transmitted wave function, i.e., $\psi(x>0)$, reads

$$\psi(x>0) \cong \sin(\pi y)e^{t\sqrt{E-x^2}x} \times \left\{1-\left[1-\frac{i}{4\pi}\ln(E_b)\frac{\sqrt{E-\pi^2}}{\sin^2(\pi\varepsilon)}\right]^{-1}\right\}, \tag{15}$$

when $E_b \equiv -4e^{-\gamma}(\pi\rho_b)^{-2}$ and thus can be identified (except for a constant) with the bound state energy of the impurity. We took in Eq. (15) only the first mode, because this is the only one that is propagating.

From Eq. (15) it is clear, that when the energy is high $[E-\pi^2 \gg \ln^{-2}(E_b)]$ the impurity has a negligible influence on the transmission, which remains to be ≈ 1. However, when $E-\pi^2 \to 0$, the transmission (T) goes to

$$T \to \frac{\ln^2(E_b)}{16\pi^2}\frac{(E-\pi^2)}{\sin^4(\pi\varepsilon)}. \tag{16}$$

Thus, $T \approx \theta^2$. When we consider a surface defect (Fig. 5), i.e., $\varepsilon \to 0$,

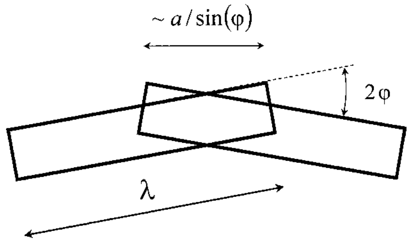

FIG. 6. The transmission through the bend can be approximated to the overlap of the localized solutions within the two rectangles.

$$T \to \frac{\ln^2(E_b)}{16\pi^6}\,\frac{(E-\pi^2)}{\varepsilon^4}. \tag{17}$$

The cause for this behavior becomes clearer when we do the following transformations:

$$\begin{aligned} y &\to (x_1-x_2)/2 \\ x &\to (x_1+x_2)/2. \end{aligned} \tag{18}$$

Now, instead of considering a single particle that propagates in a two-dimensional orifice, we can visualize two particles with coordinates x_1 and x_2 that propagate in a 1D system. That is, y stands for the distance between the particles (with a factor of 2), which cannot exceed 1, and x stands for their center of mass coordinate.

When $E-\pi^2 \to 0$, they are in their ground state, and they move like a single entity, i.e., their mutual interaction is negligible. Therefore, the exact pattern of the scattering potential is not important, and we can replace it by a 1D delta function. Thus, the problem turns to a 1D scattering problem of a single particle. This is a very simple problem, which leads to a transmission (but now an exact solution)

$$T = 1-[1+(k\rho_b)^2]^{-1}, \tag{19}$$

where k is the 1D wave number, i.e., $k \equiv \sqrt{E-\pi^2}$, and ρ_b is the de Broglie wavelength of the impurity bound state.

When $E-\pi^2 \to 0$,

$$T \to \rho_b^2(E-\pi^2). \tag{20}$$

Again, $T \approx \theta^2$.

Next, in order to explain why the change occurs *abruptly* at $\varphi \approx \theta$, we can use Fig. 6. In this figure, we see two rectangles which are relatively rotated by an angle φ. Each one of them has a length λ and a normalized width $(=1)$. We are interested in the tunneling probability of the eigenfunction $\sin(\pi y)\sin(2\pi x/\lambda)$ through the bent, which is related to the eigenvalue $\omega = \pi^2+(2\pi/\lambda)^2 = \pi^2(1+\theta^2)$.

This probability (to tunnel through the bend) is equal to the square of the overlapping integral

$$p_{\text{tunnel}} \approx \left| \int_A da\, \psi_L^* \psi_R \right|^2, \tag{21}$$

where the A stands for the overlapping area, and the subscripts L and R stand for the eigenfunctions of the left and right rectangles, respectively. This integral can be approximated to

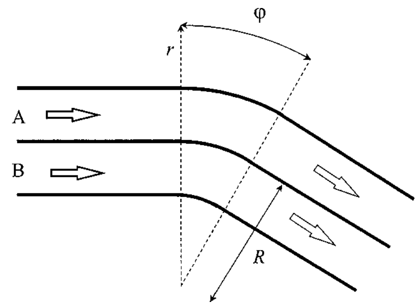

FIG. 7. Two particles enter different bent tunnels. When they penetrate the bending region particle B will suffer a stronger displacement toward the lower boundary.

$$\begin{aligned} p_{\text{turnnel}} &\approx \left| \int_{-c}^{c} dx\, \sin[\pi(x-c)/\lambda]\sin[\pi(x+c)/\lambda] \right|^2 \\ &= \left| \frac{c}{\lambda}\left[\cos(2\pi c/\lambda) - \frac{\sin(2\pi c/\lambda)}{(2\pi c/\lambda)} \right] \right|^2, \end{aligned} \tag{22}$$

where $c \cong 1/\sin\varphi$ is the overlapping *length*.

The integral (12) has a physical meaning only for $c>\lambda$, i.e., $\varphi > \overline{\varphi}_{\min} \equiv \sin^{-1}(1/\lambda) \cong \lambda^{-1}$. For $\varphi = \overline{\varphi}_{\min}$, $p_{\text{tunnel}}(\varphi = \overline{\varphi}_{\min}) = 1$, and it is decreasing down to zero very quickly. Actually, $p_{\text{tunnel}}(\varphi = 1.4\overline{\varphi}_{\min}) \approx 0$. Since, $1.4\overline{\varphi}_{\min} \cong \theta$ we have a qualitative explanation for the abrupt decline of the transmission at $\varphi \cong \theta$.

But why is there a plateau? In order to answer this question we should understand the effect of the singularity of the bend. By looking at Fig. 7 we can ask why there should be a difference between a particle that penetrates into tunnel A and another one that enters tunnel B?

Let us assume, for convenience, that in both cases the radiuses are very large $(R\to\infty)$. Then we can assume that the radial movement in the bending zone, i.e., the only radial dependence there, is $\exp(\pm i\sqrt{\omega-\pi^2}\, r\varphi)$ (where φ is the radial angle, $r \approx R$ is the radial distance and ω is the energy). It is then easy to show that the wave function in the bending zone is a superposition

$$\sin[\pi(r-R)]\left(1-\frac{r-R}{2R}\right)\left(a e^{i\sqrt{\omega-\pi^2}R\varphi} + b e^{-i\sqrt{\omega-\pi^2}R\varphi}\right), \tag{23}$$

[it was calculated to the first approximation in $(r-R)/R$].

Therefore, the probability to continue from the straight orifice to the bending part is approximately

$$\left| 2\int_R^{R+1} dr\, \sin[\pi(r-R)]^2 \left(1-\frac{r-R}{2R}\right) \right|^2 \cong 1-\frac{2}{R}. \tag{24}$$

Of course, this is only an approximated result for large radiuses, however, we can learn the tendency: the penetration probability decreases with the curvature. Even from here we see, that we should expect some problems when $R\to 0$.

Yet, we can learn another thing: as the curvature radius shrinks the particle gets closer to the origin. This behavior becomes evident from the fact that the radial wave function is not a simple $\sin[\pi(r-R)]$ but rather $\sin[\pi(r-R)][1-(r-R)/2R]$. We should expect as $R\to 0$ a singularity in the wave function itself (an evidence for this behavior we find in

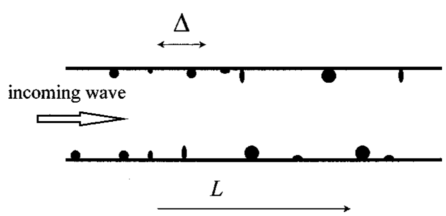

FIG. 8. Orifice with rough boundaries (the transmission is dominated by many boundaries defects).

the logarithmic divergence of the Bessel Y function). Obviously, we don't find a real divergence but instead the wave function gets a sharp peak shape. It happens since the singularity scatters all the transversal modes. As the first mode decreases all the rest increase with the same amount until the wave function has a delta function shape. Now the plateau is clear: The bending is totally transparent to a delta like incoming function, that is, once a peak shape is formed (after an angle $\varphi \approx \theta$) the bending can be increased (φ is increased) with no reduction in the transparency. This can explain the emergence of a plateau beyond the transition angle.

Before summarizing, we reckon that this picture can be implemented to transmission calculations of a rough surface orifice (for a more energetic process see Ref. 15) in the case where $\omega \to \pi^2(\theta \to 0)$. This system is illustrated in Fig. 8.

Let us, for example, assume that the spatial dimensions of the surface defects have the following distribution:

$$p(\varepsilon=\varepsilon_1)=\varepsilon_0^{-1}\exp(-\varepsilon_1/\varepsilon_0), \tag{25}$$

where p stands for the probability and ε_0 is the characteristic defect transversal location. Thus, we can apply Eq. (17) to calculate the transmission through an office with N successive surface defects

$$T=|t|^2 \cong \frac{(\theta/4)^{2N}}{(\varepsilon_1\varepsilon_2\ldots\varepsilon_N)^4}. \tag{26}$$

If we further assume, that the mean distance between successive defects is a certain Δ, Eq. (26) can be approximated to

$$T \cong \exp(-L/\xi), \tag{27}$$

where L is the distance and ξ is the localization length

$$\xi \equiv \Delta/\ln(\theta\omega_0), \quad \omega_0 \equiv 4e^{-2\gamma}/\varepsilon_0^2, \tag{28}$$

γ is the Euler's constant.

Equations (27) and (28) suggest a strong localization process due to the one-dimensional characteristic behavior of the system (in the case where $\omega \to \pi^2$).

To summarize, we have shown that when the incoming particle energy is close to the orifice threshold energy the transmission can be highly sensitive to the bending angle. We show that for every small bending angle, no matter how small is it, there is a corresponding incoming energy, below which the transmission is dropped abruptly. We also show that beyond the transition point (i.e., larger bending angles), the transmission reaches a plateau at the value $\cong \theta^2$, where θ is the transition angle.

I am grateful to Professor Mark Azbel' for enlightening discussions.

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