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Limits of convergence of the Rayleigh method for surface scattering

N. R. Hill and V. Celli
Department of Physics, University of Virginia, Charlottesville, Virginia 22901
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A method of testing the validity of the Rayleigh assumption is presented. The test can be applied for any one-dimensional or two-dimensional surface of analytic shape. It can be used for Dirichlet and Neumann boundary conditions and also when the surface is penetrable and a refracted field exists. The test is based on the asymptotic evaluation of the diffracted order amplitudes and in this way is similar to Millar's potential-theory analysis.

The problem of the diffraction of an incident plane wave from a corrugated surface is often solved by a method, described below, known as the Rayleigh method.[1] It has been shown in the case of Dirichlet boundary conditions for the sinusoidal surface $\zeta(x)=h\cos G_0x$, that the method will converge if[2] and only if[3] $G_0h<0.448$. It is useful to be able to establish convergence in more general circumstances since the Rayleigh method is often used not only for surfaces of other one-dimensional profiles, but also for two-dimensional surfaces $\zeta(x,y)$, for Neumann boundary conditions, and for cases where the surface is not impenetrable and a refracted field exists. In this note, we will give a simple, heuristic way of determining the validity of the Rayleigh method in all the cases just mentioned.

Consider the case of a plane wave, $\psi_i=e^{i\vec{k}_i\cdot\vec{r}}$, incident on a periodic surface of reciprocal-lattice vectors $\vec{G}$. For points outside of the selvedge region (i.e., outside of the region where $\zeta_{\min}<z<\zeta_{\max}$), the scattered field can be represented by an expansion in diffracted orders,

$$\sum_{\vec{G}} F_G e^{i\vec{k}_G\cdot\vec{r}} . \tag{1}$$

The wave vector of the incident wave, $\vec{k}_i=(\vec{K}_0,-p_0)$, has components parallel $(\vec{K}_0)$ and perpendicular $(-p_0)$ to the normal z direction. Likewise, the scattered wave vectors $\vec{k}_G$ are written $\vec{k}_G=(\vec{K}_G,p_G)$. They are given by the Bragg diffraction condition $\vec{K}_G=\vec{K}_0+\vec{G}$. Energy conservation gives $p_G=(k_i^2-K_G^2)^{1/2}$, where (1) tells us to take the root so that p_G is positive real for $K_G<k_i$ and positive imaginary for $K_G>k_i$.

The Rayleigh method consists of assuming that the expansion of the scattered field in diffraction orders, Eq. (1), can be analytically continued all the way back to the surface so that the coefficients F_G can be determined by the requirements of the boundary conditions. The scattered field must be analytic everywhere above the surface, including the selvedge region, because it is the solution of an elliptic differential equation.[4] It is true, then, that expansion (1) will represent the scattered field as long as the series converges. In order to test for convergence, we will derive an exact equation which expresses the expansion coefficients F_G in terms of the boundary values on the surface. Though these boundary values are not known beforehand, it is possible to determine the convergence of (1) by assuming certain analytic properties of the boundary values which are likely to hold when the surface profile $\zeta(x,y)$ is itself an analytic function.

The convergence condition. We can find the wanted expression for F_G by beginning with the exact equation for the field,[1]

$$\psi(\vec{r})=\psi_i(\vec{r})-\frac{1}{4\pi}\int\left(G(\vec{r},\vec{r}\,')\frac{\partial\psi(\vec{r}\,')}{\partial n'}-\frac{\partial G(\vec{r},\vec{r}\,')}{\partial n'}\psi(\vec{r}\,')\right)d^2S' . \tag{2}$$

The surface of integration S' is coincident with the physical surface. The normal derivative $\partial/\partial n'$ points outward from the surface. We employ a notation for the position vector $\vec{r}$ which is similar to the notation for $\vec{k}$; viz., $\vec{r}=(\vec{R},z)$. The Green's function has the integral expression[1,5]

$$G(\vec{r},\vec{r}\,')=\frac{i}{2\pi}\int d^2K\,\frac{e^{ip|z-z'|}e^{i\vec{K}\cdot(\vec{R}-\vec{R}')}}{p} ,$$

with $p=(k_i^2-K^2)^{1/2}$. Using this $G(\vec{r},\vec{r}\,')$ in (2) and taking $z>\zeta_{\max}$, we get

$$F_G=\frac{1}{2p_GA}\int_{\text{u.c.}} d^2R'\left[\exp -ip_G\zeta(\vec{R}')-i\vec{K}_G\cdot\vec{R}'\right]\times\left[H(\vec{R}')\left(p_G+\vec{K}_G\cdot\frac{\partial\zeta}{\partial\vec{R}'}\right)-L(\vec{R}')\right] . \tag{3}$$

The integral is over the unit cell which has area A. We have defined

$$H(\vec{R}')=\psi(\vec{r}')|_{z'=\zeta(\vec{R}')}\,,$$
$$L(\vec{R}')=\left(1+\left|\frac{\partial\zeta}{\partial\vec{R}'}\right|^2\right)^{1/2}\frac{\partial\psi(\vec{r}')}{\partial n'}\Bigg|_{z=\zeta(\vec{R}')}\,. \tag{4}$$

Convergence can now be determined by examining (3) as $|\vec{G}|\to\infty$. The phase $\phi(\vec{R}')=-ip_G\zeta(\vec{R}')-i\vec{K}_G\cdot\vec{R}'$ reduces to $\phi(\vec{R}')\sim|\vec{G}|\zeta(\vec{R}')-i\vec{G}\cdot\vec{R}'$ and is rapidly varying in this limit. The integral in (3) can then be evaluated by steepest descent if it is true that the quantity in braces is analytic in $\vec{R}$ for a region between the real axis and the stationary point of ϕ. We will assume that this is true and discuss this point later. The equation for the stationary point is

$$\frac{\partial\zeta(\vec{R})}{\partial\vec{R}}-i\frac{\vec{G}}{|\vec{G}|}=0\,. \tag{5}$$

The steepest descent evaluation of (3) will lead to an expression which has the exponential dependence $\exp[|\vec{G}|\zeta(\vec{R}_s)-i\vec{G}\cdot\vec{R}_s]$, where the subscript s stands for evaluation at the stationary point. The factor in (1) that multiplies F_G, $\exp[i(p_Gz+\vec{K}_G\cdot\vec{R}]$, goes like $e^{-|\vec{G}|z}$ for large $|\vec{G}|$. Hence, in order for (1) to converge at points including the lowest points in the selvedge region, it must be that

$$-|\vec{G}|\zeta_{\min}+\mathrm{Re}[|\vec{G}|\zeta(\vec{R}_s)-i\vec{G}\cdot\vec{R}_s]<0. \tag{6}$$

This gives a test for convergence: the stationary point is determined by (5) and then used in (6). Many times this can be done analytically, but even when it cannot, it is easy to solve (5) numerically for $\vec{R}_s$ and then test for convergence with (6).

The one-dimensional sinusoidal hard wall. As the first of two examples let us show that the method just described leads to the result already established for the one-dimensional profile $\zeta(x)=h\cos G_0x$.[2,3] Equation (5) gives the stationary point: $-hG_0\sin G_0x_s-i=0$. With $G_0x_s=-\sin^{-1}(i/G_0h)$ and $\zeta_{\min}=-h$, (6) then gives

$$G_0h+[1+(G_0h)^2]^{1/2}-\sinh^{-1}(1/G_0h)<0.$$

This criterion determines the maximum value of G_0h for which the Rayleigh method is valid. Putting $G_0h=(\eta^2-1)/2\eta$ we obtain Petit and Cadilhac's[3] equation for the critical value of η,

$$e^{\eta}=(\eta+1)/(\eta-1)\quad\text{or}\quad\eta=\coth\tfrac{1}{2}\eta\,.$$

This has the solution $\eta=1.543$, corresponding to $G_0h<0.448$.

The two-dimensional sinusoidal hard wall. As a second example we will examine the two-dimensional corrugated surface $\zeta(x,y)=\frac{1}{2}h(\cos G_0x+\cos G_0y)$. In this case, $\vec{G}=G_0(m\hat{x}+n\hat{y})$ can become large in different manners; that is, m or n, or both can become large. All of these cases can be handled together by putting $m=\alpha l$ and $n=\beta l$ with $\alpha=\cos\theta$ and $\beta=\sin\theta$. Then, convergence is tested for arbitrary θ as $l\to\infty$, so that $|\vec{G}|=G_0l\to\infty$ and $p_G\to iG_0l$. Equation (5) gives the stationary point,

$$G_0x_s=-\sin^{-1}\left(\frac{i\alpha}{u_0}\right),\quad G_0y_s=-\sin^{-1}\left(\frac{i\beta}{u_0}\right),$$

with $u_0=G_0h/2$. For $\zeta_{\min}=-h$, (6) gives the equation

$$2u_0+(u_0^2+\alpha^2)^{1/2}+(u_0^2+\beta^2)^{1/2}-\sinh^{-1}(\alpha/u_0)-\sinh^{-1}(\beta/u_0)=0 \tag{7}$$

for the critical value of u_0. Roots u_0 of (7) are found numerically for values of θ between 0° and 45°, which is sufficient in this case because of the symmetry of the surface. The smallest of the roots is the overall critical value for this two-dimensional surface. The value is found to be $2u_0=G_0h=0.592$. This is the root that occurs at $\theta=0°$.

The Rayleigh method has been applied to calculate the scattering of He from a LiF (001) surface.[6-8] The surface parameter h is varied in order to match experimental data. The unit cell of the surface is a square of side 2.84 Å, giving $G_0=2.21$ Å^{-1}. This implies that h should not be larger than $h=0.268$ Å if there is to be strict convergence. Although this condition is often not met (e.g., $h=0.305$,[6] and[7] $h=0.295$), it is still probably true that the Rayleigh method gives good asymptotic results. That is, the boundary conditions can be satisfied to a good approximation with a finite number of terms in the expansion even though the expansion eventually diverges.

Analytic properties of the boundary values. The analysis above is based on the assumption that the boundary values $H(\vec{R})$ and $L(\vec{R})$ are analytic from the real axis to the stationary point. We asserted that this is likely to hold when the profile $\zeta(\vec{R})$ is an analytic function. This can be seen by examining the self-consistent equations[9] for boundary values when either Dirichlet or Neumann conditions hold:

For Dirichlet conditions, with P denoting principal value,

$$\frac{\partial\psi(s)}{\partial n}=2\left(\frac{\partial\psi_i(s)}{\partial n}-\frac{1}{4\pi}\,\mathrm{P}\int\frac{\partial G(s,s')}{\partial n}\times\frac{\partial\psi(s')}{\partial n'}\,ds'\right)\,. \tag{8}$$

For Neumann conditions,

$$\psi(s)=2\left(\psi_i+\frac{1}{4\pi}\,\mathrm{P}\int\frac{\partial G(s,s')}{\partial n'}\,\psi(s')\,ds'\right)\,. \tag{9}$$

Both s and s' denote points on the surface; i.e., s means $\vec{r}=(\vec{R},\zeta(\vec{R}))$. The kernel of (8),

$$\frac{\partial G(s,s')}{\partial n}=\frac{\partial}{\partial n}\left(\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\right)_{z=\zeta(\vec{R}),\ z'=\zeta(\vec{R}')},$$

is an analytic function for real values of $\vec{R}\neq\vec{R}'$ if $\zeta(\vec{R})$ is an analytic function. Since the point $\vec{R}=\vec{R}'$ is excluded from the integral, we can conclude that $\partial\psi(s)/\partial n$ is analytic for real $\vec{R}$. Moreover, it will remain analytic as $\vec{R}$ takes on complex values if $|\vec{r}-\vec{r}'|$ is never zero as $\vec{R}'$ ranges over its (real) values of integration. We will not pursue this point any further. For the case of a simple sinusoid $\zeta(x)=h\cos G_0x$, Millar[2] rigorously shows that the stationary point and the real axis lie within an analytic strip.

Nonanalytic profiles. When the surface profile $\zeta(\vec{R})$ is not analytic, (3) cannot be evaluated by steepest descent so that special considerations are needed to discuss the validity of the Rayleigh assumption. If the surface has sharp corners, the field will usually be singular at the corners.[10] If the field is singular, then by a theorem given by Millar[2], the Rayleigh assumption is invalid. It should be pointed out, though, that under special circumstances, the field is not singular at a corner and the Rayleigh method provides an exact solution. Meecham[11] gives an example of this: for an echelette surface with Neumann boundary conditions the incidence angle and the incident wavelength can be chosen so that the Rayleigh series (1) terminates after only one term.

A nonanalytic profile can be approximated by a truncated Fourier expansion, an analytic function, so that the method of this paper can be applied. We did this for a symmetric sawtooth for which only odd cosine terms appear in the Fourier expansion of $\zeta(x)$. For $G_0h=0.1$, where G_0 is the fundamental and $2h$ is the peak-to-peak amplitude, the convergence test, (5) and (6), indicates that the Rayleigh method is valid when $\zeta(x)$ is represented by the first 10 odd cosine terms and invalid when $\zeta(x)$ is represented by 15 terms.

Penetrable surfaces. The Rayleigh method is often used when a refracted field exists. In this case the refracted field is also expanded in diffracted orders,[1,12]

$$\sum_{\vec{G}} F'_G e^{i\vec{k}'_G\cdot\vec{r}}\ . \tag{10}$$

The vectors $\vec{k}'_G$ are determined by the Bragg condition so that $\vec{k}'_G=(\vec{K}_G,-q_G)$ where $q_G=(\epsilon k_i^2-K_G^2)^{1/2}$. Equations (1) and (10) are extended to the surface from above and below, and boundary conditions are applied in order to find F_G and F'_G. The analysis already used to determine the convergence of (1) still applies. We can go through the same analysis for (10), only using the Green's function $G'(r)=e^{ik'r}/r$, where $k'=k\epsilon^{1/2}$ (see Ref. 1). Since $q_G\to i|\vec{G}|$ when $|\vec{G}|\to\infty$ and since (10) must converge up to the highest point within the material $\zeta_{\max}$, the convergence of (10) is determined by the equations

$$\frac{\partial\zeta}{\partial\vec{R}}+\frac{i\vec{G}}{|\vec{G}|}=0\ , \tag{11}$$

$$|G|\,\zeta_{\max}+\mathrm{Re}[-|\vec{G}|\,\zeta(R_s)-i\vec{G}\cdot\vec{R}_s]<0\ . \tag{12}$$

Just as in (5) and (6), Eq. (11) is used to determine the stationary phase point, and then convergence is tested by (12). In particular, the convergence criterion is independent of ϵ.

Conclusion. When the Rayleigh assumption is valid, a simple, exact calculation of the scattering from a periodic surface is allowed. A rigorous criterion for its validity has been known for some time in the case of a simple sinusoidal surface.[2,3] We have given a method of testing the assumption's validity when it is applied to any analytically shaped surface. The first steps of this test, the application of Eqs. (5) and (6), are easily carried out, and one can usually stop here and have a high degree of confidence of the validity of the Rayleigh assumption for a particular surface. In the case of Dirichlet or Neumann boundary conditions, one can go on and rigorously establish the validity by examining the locations of the singularities in the kernel of (8) or (9).

Even if the Rayleigh assumption is invalid, the general method of calculation can sometimes be judiciously applied to get good asymptotic results. Also, it is now known[13] that when the coefficients (1) are calculated by a variational procedure,[11] an exact solution is obtained.

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[1]For a comprehensive list of references, see F. Toigo, A. Marvin, V. Celli, and N. R. Hill, Phys. Rev. B 15, 5618 (1977). We employ the same notation as in this reference.

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