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1980 J. Phys. A: Math. Gen. 13 1433

(http://iopscience.iop.org/0305-4470/13/4/032)

J. Phys. A: Math. Gen. **13** (1980) 1433–1441. Printed in Great Britain

Theory of the scattering of electromagnetic waves by a regular grid of parallel cylindrical wires with circular cross section

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Received 23 April 1979, in final form 24 August 1979

Abstract. A method is described for calculating the scattering of electromagnetic waves by a grid of equally spaced parallel cylindrical wires with finite conductivity. It is an adaptation of the 'Green function' method used in solid-state band-structure theory, as described by Ham and Segall. In this paper the theory is restricted to the case when the direction of incidence is in a plane perpendicular to the wires. Curves are shown for the transmission at normal incidence in situations typical of infrared spectroscopy.

1. Introduction

The use of wire-grid beam splitters in interferometers has led to experimental studies of their optical characteristics in the far-infrared range of frequencies. These grids consist of a set of equally spaced parallel wires. The theory of such grids has been attempted in many ways, such as those reviewed by Larsen (1962) and Petit (1975). We describe yet another method, which has been used to check experimental results obtained by dispersive Fourier transform spectrometry (Mok *et al* 1979). In this article we describe the theory only for waves incident perpendicular to the axes of the wires. We plan in a later article to extend the theory to the case of arbitrary incidence.

The method is based on the 'Green function' method of solid-state band-structure theory (Ham and Segall 1961). The wave equation is transformed into an integral equation with a Green function for kernel. The integral can be turned into a surface integral over the surface of one of the wires, and the integral equation is then turned into a matrix problem by the use of partial-wave expansions. Since the Green function does not involve the scatterer, it does not need to be recomputed if the radius of the scatterer is varied. It is assumed that the wires have a circular cross section. Presumably methods such as those of Waterman (1973) and Barber (1977) could be adapted to deal with more general cases.

The method works well when the diameter of the wires does not greatly exceed the wavelength of the incident radiation and when it is less than about 80% of the spacing. These conditions are well satisfied in normal conditions.

0305-4470/80/041433+09$01.50

The use of Green functions in a fairly general context is described by Morse and Feshbach (1953) and Jackson (1962). Bessel and Hänkel functions and their integral representations are discussed by Watson (1944), Abramowitz and Stegun (1965) and Gradshteyn and Ryzhik (1965).

2. Basic equations

The basic method is described by Ham and Segall (1961). There the problem concerns wave propagation through a three-dimensional lattice of non-absorbent spheres. We consider a plane grid of identical, parallel, equally spaced cylindrical wires of radius c, and with a period a ($a > 2c$). The axis of one of the wires is chosen as the z axis and the x axis is taken also in the plane of the grid (figure 1). The wires are made of a substance of

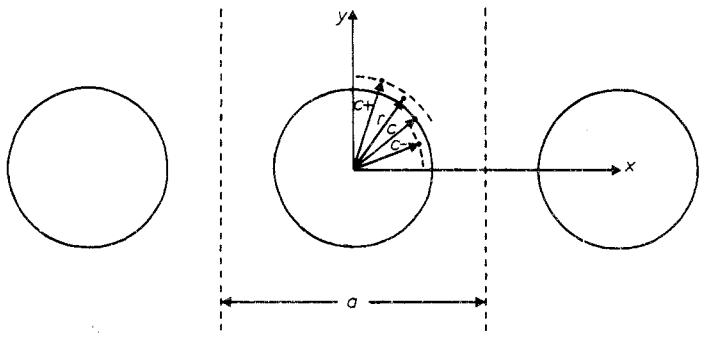

Figure 1. To illustrate the radial distances $c-$, c, r, and $c+$, and a unit 'cell' $|x| < \frac{1}{2}a$. In the end the limits $c- \to c$, $c+ \to c$ are taken, with r trapped between c and $c+$.

conductivity σ. The direction of the incident radiation lies in the Oxy plane. Then we need consider only two directions of polarisation, one with the electric vector $\boldsymbol{E}$ parallel to the wires, and the other with the magnetic vector $\boldsymbol{B}$ parallel to the wires. In the case of monochromatic radiation, with a time variation taken as $e^{-i\omega t}$, the Maxwell equations reduce to the form

$$-\nabla^2\psi(\boldsymbol{r}) + V\psi(\boldsymbol{r}) = \kappa^2\psi(\boldsymbol{r}) \tag{1}$$

with $\boldsymbol{r} = (x, y)$, $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$, and $\kappa = \omega(\epsilon_0\mu_0)^{1/2}$. In the former case the dependent variable ψ is E_z and V is equal to $-i\omega\mu_0\sigma$; in the latter the dependent variable is B_z and V is a more complicated gradient operator (see (25) below). Except that V may be complex this equation has the same form as the Schrödinger equation of band-structure theory. It should be noted that V vanishes outside the wires. In order to put in the boundary condition that the scattered waves are outgoing it is convenient to give κ^2 a small positive imaginary part, which is allowed to tend to zero at the end.

With an incident wavevector (k_0, l_0) with $l_0 = (\kappa^2 - k_0^2)^{1/2}$ we choose the incident wave as

$$b_0(\boldsymbol{r}) = l_0^{-1/2} \exp[i(k_0 x + l_0 y)].$$

The diffracted plane wave will be taken as

$$b_m(\boldsymbol{r}) = |l_m|^{-1/2} \exp[i(k_m x + l_m y)]$$

with $k_m = k_0 + 2\pi m/a$, $l_m = \pm_m(\kappa^2 - k_m^2)^{1/2}$. The factor $|l_m|^{-1/2}$ is put in so that unit amplitude corresponds to unit power. The suffix m should be regarded as composite, with an integer part to specify the order of diffraction and a two-valued part to specify the sign of l_m.

The free-space Green function satisfies

$$(\kappa^2 + \nabla'^2)G_0(\boldsymbol{r} - \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{2}$$

and is given by

$$G_0(\boldsymbol{R}) = -\tfrac{1}{4}\,\mathrm{i}H_0(\kappa R)$$

where H_0 is a Hänkel function of the first kind. We use $\boldsymbol{R}$ for $\boldsymbol{r} - \boldsymbol{r}'$, with components X, Y. We need the Green function satisfying

$$G(X + a,\ Y) = \exp(\mathrm{i}k_0 a)G(X,\ Y)$$

which is given by

$$G(\boldsymbol{R}) = -\tfrac{1}{4}\,\mathrm{i}\sum_{s=-\infty}^{\infty} H_0(\kappa|\boldsymbol{R} - \boldsymbol{a}s|)\exp(\mathrm{i}k_0 as) \tag{3}$$

with $\boldsymbol{a} = (a, 0)$. An alternative expression is given by the Fourier expansion:

$$G(X,\ Y) = (2\pi a)^{-1}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}l(\kappa^2 - l^2 - k_n^2)^{-1}\exp[\mathrm{i}(k_n X + lY)]$$

with $k_n = k_0 + 2\pi n/a$ and with κ^2 having a small imaginary part. For large positive values of Y the method of residues shows that $G(X, Y)$ is given approximately by

$$G(X,\ Y) \approx -(2\pi a)^{-1}\sum_m{}'' \ \pi\,\mathrm{i}|l_m|^{-1}\exp[\mathrm{i}(k_m X + l_m Y)]$$

where the sum is taken over those values of m giving real positive values of l_m. Thus we obtain for $y \gg y'$:

$$G(\boldsymbol{r} - \boldsymbol{r}') \approx -\mathrm{i}(2a)^{-1}\sum_m{}'' \, b_m(\boldsymbol{r})\, b_m^*(\boldsymbol{r}'). \tag{4}$$

There is a similar result for $y' \gg y$.

From now on we may consider $\boldsymbol{r}$ and $\boldsymbol{r}'$ as being restricted to a single 'cell' $|x| < \frac{1}{2}a$ (figure 1). Equation (1) may be transformed into the integral equation

$$\psi(\boldsymbol{r}) = b_0(\boldsymbol{r}) + \int \mathrm{d}^2\,\boldsymbol{r}' G(\boldsymbol{r} - \boldsymbol{r}')V(\boldsymbol{r}')\psi(\boldsymbol{r}') \tag{5}$$

where the 'volume' of integration should be a whole cell, but since $V(\boldsymbol{r}')$ vanishes for $r' > c$, it may be taken to be the 'volume' inside $r' = c+$ where $c+$ is a fixed quantity between c and $\frac{1}{2}a$, but usually taken to be just greater than c (figure 1). Hence, for y large and positive we find by (4) that

$$\psi(x,\ y) \approx \sum_m{}'' \, S_{m0} b_m(x,\ y)$$

with

$$S_{m0} = \delta_{m0} - \mathrm{i}(2a)^{-1}\int_{r' \leqslant c+} \mathrm{d}^2\boldsymbol{r}' b_m^*(\boldsymbol{r}')V(\boldsymbol{r}')\psi(\boldsymbol{r}') \tag{6}$$

and similarly for negative values of y. The S_{m0} are the required scattering amplitudes

and when there is no absorption it can be numerically verified that they satisfy the energy conservation rule:

$$\sum_m |S_{m0}|^2 = 1. \tag{7}$$

3. Partial-wave expansions

In order to find S_{m0} we need to determine $G(\boldsymbol{r}-\boldsymbol{r}')$ from (3), say, and then use it in (5) to get $\psi(\boldsymbol{r})$, which is then in turn used in (6). To facilitate this process we expand b, ψ and G in partial waves, but before doing this it is convenient to turn the integrals in (5) and (6) into surface integrals.

Because of (1) we may replace $V(\boldsymbol{r}')$ in (6) by $(\kappa^2+\nabla'^2)$. Then we replace $\kappa^2 b(\boldsymbol{r}')$ by $-\nabla'^2 b(\boldsymbol{r}')$, and use Green's theorem to obtain

$$S_{m0} = \delta_{m0} - \mathrm{i}(2a)^{-1} \int_{r'=c+} \mathrm{d}S' \left(b_m^*(\boldsymbol{r}') \frac{\partial}{\partial r'} \psi(\boldsymbol{r}') - \psi(\boldsymbol{r}') \frac{\partial}{\partial r'} b_m^*(\boldsymbol{r}') \right). \tag{8}$$

A similar idea is used for (5) but we first choose $\boldsymbol{r}$ so that $r < r'$ (figure 1). By (2) we have $\kappa^2 G = -\nabla'^2 G(\boldsymbol{r}-\boldsymbol{r}') + \delta(\boldsymbol{r}-\boldsymbol{r}')$ and so we obtain, after cancelling $\psi(\boldsymbol{r})$ from each side,

$$b(\boldsymbol{r}) = \int_{r'=c+} \mathrm{d}S' \left(\psi(\boldsymbol{r}') \frac{\partial}{\partial r'} G(\boldsymbol{r}-\boldsymbol{r}') - G(\boldsymbol{r}-\boldsymbol{r}') \frac{\partial}{\partial r'} \psi(\boldsymbol{r}') \right). \tag{9}$$

For the expansions we introduce orthonormal angle-dependent functions:

$$Y_l(\boldsymbol{r}) = (2\pi)^{-1/2} \exp(\mathrm{i}l\theta_r) \tag{10}$$

(where θ_r is the polar angle of $\boldsymbol{r}$ and $l = 0, \pm 1, \pm 2, \ldots$) or similar sine and cosine functions which enable us to exploit the symmetry of the structure under $y \leftrightarrow -y$. Then we expand in solutions of the appropriate wave equations separated in polar coordinates:

$$b_m(\boldsymbol{r}) = \sum_{l=-\infty}^{\infty} b_l^{(m)} J_l(\kappa r) Y_l(\boldsymbol{r}) \tag{11}$$

$$\psi(\boldsymbol{r}) = \sum_l \psi_l \phi_l(\kappa, r) Y_l(\boldsymbol{r}) \tag{12}$$

$$G(\boldsymbol{r}-\boldsymbol{r}') = \sum_l Y_l(\boldsymbol{r}) Y_l^*(\boldsymbol{r}') (-\tfrac{1}{2}\mathrm{i}\pi) J_l(\kappa r_<) H_l(\kappa r_>)$$

$$-\tfrac{1}{2}\mathrm{i}\pi \sum_{ll'} D_{ll'} Y_l(\boldsymbol{r}) Y_{l'}^*(\boldsymbol{r}') J_l(\kappa r) J_{l'}(\kappa r'). \tag{13}$$

Here the J_l are Bessel functions and the ϕ_l are the solutions of the radial equation obtained from (1). The coefficients $b_l^{(m)}$ are obtained from the expansion

$$\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}) = 2\pi \sum_l \mathrm{i}^l J_l(\kappa R) Y_l^*(\boldsymbol{k}) Y_l(\boldsymbol{R}) \tag{14a}$$

as

$$b_l^{(m)} = 2\pi \mathrm{i}^l |l_m|^{-1/2} Y_l^*(\boldsymbol{k}_m). \tag{14b}$$

In (11)–(14) the summations over l and l' are taken from $-\infty$ to $+\infty$. The quantities $r_>$ and $r_<$ are the greater and lesser, respectively, of r and r'. The first part of G is the

expansion of G_0 which can be derived by adapting a method described by Jackson (1962), as can (14*a*). The rest of G can be regarded as being produced by the sources in (3) other than that for $s = 0$, and the coefficients $D_{ll'}$ have yet to be determined.

The angular integrals in (8) and (9) are performed using the orthonormality of the $Y_l(\boldsymbol{r}')$ to give, after eliminating the coefficients ψ_l,

$$S_{n0} = \delta_{n0} - (\pi a)^{-1} \sum_{ll'} b_l^{*(n)} (M^{-1})_{ll'} b_{l'}^{(0)} \tag{15}$$

with

$$M_{ll'} = D_{ll'} + p_l \delta_{ll'} \tag{16}$$

where

$$p_l = [(H_l \phi_l' - \phi_l H_l')(J_l \phi_l' - \phi_l J_l')^{-1}]_{r'=c+} \tag{17}$$

the primes denoting $\mathrm{d}/\mathrm{d}r'$. We have let r in (9) tend to r' from below.

4. Computation of the Green function

The coefficients $D_{ll'}$ in (13) and (16) are related to the coefficients B_L in the expansion

$$G(\boldsymbol{R}) = -\tfrac{1}{4}\mathrm{i} H_0(\kappa R) + \sum_L \mathrm{i}^L B_L J_L(\kappa R) Y_L(R) \tag{18}$$

by

$$D_{ll'} = \mathrm{i}^{l-l'} 4\mathrm{i} \sum_L C_{ll'}^L B_L \tag{19a}$$

with

$$C_{ll'}^L = \int_{q=1} \mathrm{d}S_q Y_l^*(\boldsymbol{q}) Y_{l'}(\boldsymbol{q}) Y_L(\boldsymbol{q}) \tag{19b}$$

(which is simply $(2\pi)^{-1/2}\delta_{L,l-l'}$ if the Y_l are given by (10)). This result can be obtained by expanding each exponential in $\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}) = \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r})[\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}')]^*$ by (14*a*) and integrating round a circle in the $\boldsymbol{q}$ plane centred on the origin to give an expansion for $J_L(qR)Y_L(\boldsymbol{R})$.

To obtain the B_L we may use a technique suggested by Ham and Segall (1961). The Hänkel functions in (3) are replaced by an integral representation, which is broken into two ranges at a real value α of the argument. One part can be summed by Fourier methods, and the other is left as it is. The technique gives a swiftly convergent expression for $G(\boldsymbol{R})$. Then the limit $\boldsymbol{R} \to 0$ is taken. With the definition (10) we finally obtain

$$B_L = -(2\pi)^{-1/2} \kappa^{-|L|} (X_1 + X_2 + X_3) \tag{20}$$

with

$$X_1 = a^{-1} \sum_{n=-\infty}^{\infty} \int_0^{\infty} \mathrm{d}l \, [2\,\mathrm{Re}(k_n - \mathrm{i}l)^{|L|}] (k_n^2 - \kappa^2 + l^2)^{-1} \exp[-(k_n^2 - \kappa^2 + l^2)(4\alpha^2)^{-1}] \tag{21a}$$

$$X_2 = \sum_{s=1}^{\infty} 2\cos(k_0 as - \tfrac{1}{2}\pi|L|) \int_{\alpha}^{\infty} \mathrm{d}\xi \, \xi^{-1} (2\,as\,\xi^2)^{|L|} \exp[\kappa^2 (4\xi)^{-2} - a^2 s^2 \xi^2] \tag{21b}$$

$$X_3 = \tfrac{1}{2}\delta_{L0} \int_{-\infty}^{\kappa^2(4\alpha^2)^{-1}} \mathrm{d}y (y + \mathrm{i}0)^{-1} \mathrm{e}^y. \tag{21c}$$

We note that $B_{-L} = B_L$. Here the quantity α is a real and positive parameter, which affects the rate of convergence of (21) but not the final result. The quantity $+\mathrm{i}0$ in (21*c*) is to indicate that the pole is to be avoided by passing above it. A sketch for a proof is given below.

A less elaborate but rather slowly convergent formula is obtained as follows. As in (13) we may set, for $s \neq 0$,

$$G_0(\boldsymbol{R} - \boldsymbol{a}s) = \sum_l Y_l(\boldsymbol{R}) Y_l^*(\boldsymbol{a}s)(-\tfrac{1}{2}\mathrm{i}\pi) J_l(\kappa R) H_l(\kappa a|s|). \tag{22}$$

Next we put $G(\boldsymbol{R}) = G_0(\boldsymbol{R}) + \bar{G}(\boldsymbol{R})$, so that

$$\bar{G}(\boldsymbol{R}) = \sum_{s \neq 0} G_0(\boldsymbol{R} - \boldsymbol{a}s) \exp(\mathrm{i}k_0 as). \tag{23}$$

If we then substitute (22) into (23) and compare with (18) we obtain

$$B_L = -(2\pi)^{-1/2} \mathrm{i}\pi \sum_{s=1}^{\infty} H_{|L|}(\kappa as) \cos(k_0 as - \tfrac{1}{2}\pi|L|). \tag{24}$$

This result may be used to demonstrate the correctness of (20) and (21). First, by differentiating with respect to α under the integral sign we may show that the result is independent of α. Then we manoeuvre α in the complex plane towards zero so that X_1 and X_3 tend to zero. (For this to be successful κ^2 must have a positive imaginary part, so that $\arg(\kappa^2)$ is just greater than 0, and then $\arg(\alpha)$ must lie between $-\frac{1}{4}\pi$ and $-\frac{1}{4}\pi + \frac{1}{2}\arg(\kappa^2)$, see Ham and Segall 1961). Then the integrals in X_2 become integral representations of the Hänkel functions in (24).

Formula (24) converges very slowly, but quite good answers can be produced by careful 'apodisation' and the correctness can be checked against (20) and (21). The imaginary part of B_L is best obtained from (21*a*) and (21*c*) from the poles just off the real axis; there is no contribution from (21*b*).

Several checks for program correctness are available. First, if (20) and (21) are used the results should not depend on α. Secondly the results should agree with (24). Thirdly, with zero dissipation in the wires the sum rule (7) can be used. Finally, if the scatterers are weak the 'Born approximation' (Morse and Feshbach 1953) can be used by replacing ψ in (6) by b and performing the integral directly without using G.

5. The amplitudes at the wire

We now discuss how to find the logarithmic derivatives of the radial functions at the surface of the wire, i.e. $(\mathrm{d}\phi_l/\mathrm{d}r)\phi_l^{-1}$ evaluated at $r = c+$. This quantity is needed for (17) and, in fact, is the way in which the properties of the wire enter the theory.

In the case with $\boldsymbol{E}$ parallel to the wires the wave equation is (with $\psi = E_z$)

$$\nabla^2 \psi = Q\psi$$

with

$$Q = -\mathrm{i}\omega\mu_0\sigma - \omega^2\epsilon_0\mu_0.$$

We define $q = Q^{1/2}$, with the sign chosen so that $\mathrm{Re}(q) > 0$. Inside a metal at infrared

frequencies the second term in Q may be neglected, so that $q = (\omega\mu_0\sigma)^{1/2} \exp(-\frac{1}{4}i\pi)$. In free space we let $\sigma \to 0+$ in Q, so that $q = -i\omega(\epsilon_0\mu_0)^{1/2}$. Then it is found that both ψ and $d\psi/dr$ are continuous across the interface, so that

$$[\phi_l'/\phi_l]_{r=c+} = \{[dJ_l(iqr)/dr]/J_l(iqr)\}_{r=c-}$$

with $c+$ just greater than c, and with $c-$ just less than c. Thus we evaluate this expression using the radial function just inside the wire.

In the case of infrared radiation incident at 3 THz on tungsten ($\sigma^{-1} = 55 \times 10^{-9}\Omega$ m) the skin depth is about 0·1 μm, which is very much less than a typical wire diameter of 5–10 μm. Thus we approximate ϕ_l by e^{qr}, so that

$$(\phi_l'/\phi_l)_{r=c+} \approx q.$$

For the other polarisation we put $\psi = B_z$ to give the wave equation

$$\nabla \cdot (Q^{-1}\nabla\psi) = \psi \tag{25}$$

from which it follows that $Q^{-1}\partial\psi/\partial r$ (as well as ψ) is continuous across the interface. (This can be transformed into the form (1) with V replaced by $[\kappa^2 + Q - Q\nabla(Q^{-1}) \cdot \nabla]$, the third term of which is a first-order differential operator.) Hence we find that

$$(\phi_l'/\phi_l)_{r=c+} = [Q(c+)/Q(c-)]\{[dJ_l(iqr)/dr]/J_l(iqr)\}_{r=c-}.$$

With the above approximation this gives

$$(\phi_l'/\phi_l)_{r=c+} \approx -\omega^2\epsilon_0\mu_0/q.$$

6. Uses of symmetry

Although it is more convenient to use the definition (10) of Y_L for the expansion (18), a different definition is better in (11)–(13). One may replace l by a composite suffix lm ($l \geqslant m \geqslant 0$) and set $Y_{00} = (2\pi)^{-1/2}$, and for $l > 0$, $Y_{l0} = \pi^{-1/2} \cos l\theta_r$, $Y_{l1} = \pi^{-1/2} \sin l\theta_r$. Equations (14) and (19) are still valid, but the functions Y_L are now distinct from Y_l and $Y_{l'}$. Then it is found that the matrix elements $M_{lm,l'm'}$ in (16) vanish for $m \neq m'$, so that the matrix separates into two parts, one for $m = 0$ and the other for $m = 1$. This reduction is associated with reflection symmetry in the plane of the grid. When the radiation is normally incident there is a further increase in symmetry. It follows from (24) that B_L vanishes for L odd, so that by (19) $M_{lm,l'm'}$ vanishes if $(l - l')$ is odd. Thus $M_{lm,l'm'}$ is further reduced into parts with l, l' even, and l, l' odd. Moreover, by (14b) $b_l^{(0)}$ vanishes if $l - m$ is odd, so that for $m = 0$ we need only take l, l' even, and for $m = 1$ l, l' odd.

7. Some results

A few curves of the transmission amplitude against frequency are shown in figure 2 for five values of the wire diameter. The period a is taken as 100 μm and the radiation is assumed to fall normally on the grid, with the E vector parallel to the wires. The transmission amplitudes are not affected by more than a few per cent even when the resistivity is increased a hundred times, so that as expected these curves are very close to

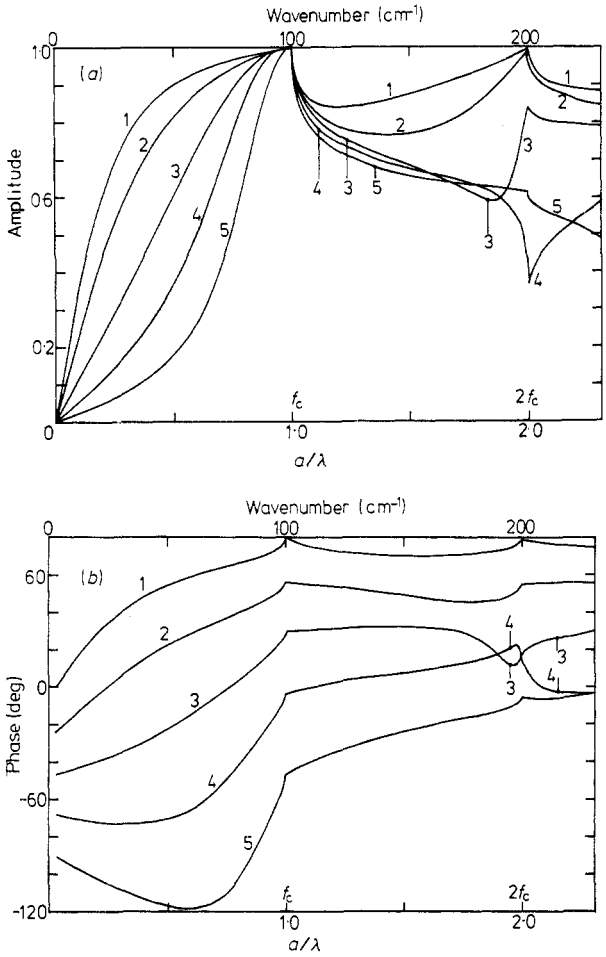

Figure 2. Plots of the transmission amplitude (*a*) and phase (*b*) against frequency for wires of diameter (1) 5μm, (2) 10μm, (3) 20μm, (4) 30μm, (5) 40μm. The spacing, *a*, is 100μm and the resistivity of the wires is $55 \times 10^{-9}\Omega$m. The critical frequency is 100 cm^{-1} or 3 THz. λ is the wavelength. It should be noted that on the phase diagram the vertical scale is correct for curve (5), but that to avoid confusion, curves (1), (2), (3) and (4) have been displaced upwards by 80, 60, 40 and 20°, respectively.

the ideal case. (However, the reflectivities are more significantly reduced by an increase in the resistivity.)

The curves show that at the first critical frequency the transmission becomes almost perfect. The theory is not straightforward at these frequencies because the coefficients B_L of the Green function in (20) have a 'reciprocal square root' divergence coming from the vanishing of the denominator in (21*a*) at zero argument when $k_n = \kappa$. However, for thin wires ($c \ll 2\pi/\kappa$) only the partial wave with $l = 0$ is significant. In this case the matrix M in (15) is simply a scalar, and its divergence causes the second term to vanish, so that $S_{00} = 1$. It seems that the first diffracted waves, moving parallel to the grid, with a wavelength matching the spacing, can set themselves so that at the wires they almost completely cancel the incident wave. We have not investigated why this seems to

happen with thicker wires, at least at the first critical frequency, but it may be a consequence of the use of the approximate formula (24) for the Green function, which cannot give the divergence correctly at the critical frequencies.

In this paper we have given a method for calculating the scattering of electromagnetic radiation from a grid of parallel wires. In a subsequent paper we intend to use this method to study the performance of interferometers constructed with wire-grid beam dividers and polarisers (Martin and Puplett 1970).

Acknowledgments

C L Mok is indebted to SRC for the award of a CASE postgraduate research studentship. The authors also wish to thank the University of London and Westfield College Computing Centres for the use of their facilities and the Numerical Algorithms Group for the use of their subroutines.

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