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Formally closed solution for a crystal with spatial dispersion

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A formally closed solution is exhibited for a semi-infinite spatially dispersive crystal, with point-dipole harmonic oscillators located at the crystal sites, and s-polarized incident light. The dipole interactions, including retardation, are taken into account exactly, and observable quantities may be calculated with arbitrary accuracy without great computational effort. The method requires the summing of a rapidly converging series, followed by a contour integral around the unit circle. Some numerical results are presented, and a comparison made with standard approximate methods. The case of p-polarized light is postponed to a future publication.

I. INTRODUCTION

Since the original discussion by Pekar[1] of the phenomenon of spatial dispersion, much of the theoretical work has centered on the problem of the so-called additional boundary conditions (ABC's), which appear to be required to determine reflection and transmission coefficients, etc., of a spatially dispersive crystal.[2] In Pekar's original work, the additional boundary condition was chosen in a rather arbitrary way. In recent years, there have been a number of attempts, notably through what is known as the dielectric approximation,[3,4] to obtain correct boundary conditions from a knowledge of the bulk dielectric properties of the substance, without recourse to additional, arbitrary assumptions. The dielectric approximation, however, has recently been criticized by several authors.[5-8]

In view of this state of affairs, it seems worthwhile and appropriate to adopt a microscopic approach, in which one attempts to solve the Maxwell equations for the actual crystal, or at least a more or less realistic model thereof. One such model was proposed some years ago by Deutsche and the present author,[9] but it involved the rather restrictive assumption that bare exciton eigenfunctions in a semi-infinite crystal were taken to be exactly sinusoidal, necessitating in most cases a distortion of the interactions near the crystal surface. In another model, due to Mahan and Obermair,[10] one treats the interaction between a crystal plane and its N nearest neighbors exactly, neglecting the others. This approach has found a number of applications, notably by Philpott.[11] In practice, because of computational difficulties and because the error committed is in any case usually not great, N is usually taken to be zero or one.

More recently, it has been discovered that the Maxwell equations are exactly soluble if the interaction between crystal planes is assumed to fall off exponentially with distance, and this "exp model" has been studied by several authors.[6,7,12]

The actual dipolar interaction between crystal planes is known to fall off with distance as an infinite sum of exponentials.[13,14] Thus, one expects that both the Mahan-Obermair method with $N=1$ and the exp model should be at least qualitatively correct, and indeed this appears to be the case. However, neither approximation is quantitatively accurate for all cases, and attempts to improve them systematically lead to rapidly increasing computational difficulties. For N nearest neighbors, one must solve an $(N+1)$st-order equation for $N+1$ refractive indices. Essentially the same thing happens if one tries to improve the exp model by including N exponentials instead of only one. Another (usually minor) problem is that in both methods the dipolar interactions is normally taken to be instantaneous, so that retardation is not really included correctly.

The purpose of the present paper is to point out that, at least for s polarization, all these difficulties can be avoided, as there exists a relatively simple, formally closed solution. In order to avoid misunderstanding, we state here just what we mean by "formally closed." Our model is a semi-infinite crystal, with the sites occupied by point-dipole harmonic oscillators. The incident light must be s polarized, but may have any angle of incidence. The calculation of any desired observable (reflection coefficient, polarization at any desired site, electric field at any point) is then reduced to two steps: first, the evaluation of a function of a complex variable defined by a rapidly converging infinite series; second, doing a contour integral with this function around the unit circle. One can achieve any desired degree of accuracy simply by accurate series summation and subsequent integration. Retardation is taken into account exactly. We will only give the treatment for a simple cubic crystal, but it will be obvious

that this is not a real limitation.

In our approach, we abandon the attempt to describe the crystal in terms of refractive indices, since both the number of different ones of these and their numerical values are highly model sensitive. In both the Mahan-Obermair and exp methods, the number of refractive indices turns out to be $N+1$, where N is the number of nearest-neighbor planes, or the number of exponentials, included. Moreover, the numerical values of these many refractive indices are quite different for the two models,[7] so it would seem that they have little real significance. Instead, we deal directly with observable properties, with the key observable in our approach being the polarization as a function of site location.

The author is confident that similar methods will be able to deal with the case of p polarization as well. This case is more complicated, however, so its consideration will be postponed to a later paper.

In Sec. II, we set up the problem in a form suitable for our approach, and the actual solution is presented in Sec. III. In Sec. IV, there is some discussion, notably of the limits of validity of the one-near-neighbor and exp approximation. A few numerical results are presented, and compared with the results of approximate methods.

II. FORMULATION

Much of the content of this section is equivalent to work which is to be found in Refs. 11, 13, and 14. It is nevertheless recapitulated here for completeness and to obtain it in a form suitable for our purposes.

We consider a semi-infinite, simple cubic crystal with the unit of length chosen equal to the distance between neighboring sites. Point-dipole harmonic oscillators are located at all sites with $x,y=0,\pm1,\pm2,\ldots$, and $z=1,2,3,\ldots$. We use the symbol $\vec{l}$ to denote the vector location of an occupied site. The unit of time is chosen such that the velocity of light $c=1$.

The electromagnetic field will be described by the Hertz vector $\vec{U}$ satisfying the equation

$$\ddot{\vec{U}} - \nabla^2\vec{U} = 4\pi\vec{P}, \tag{1}$$

with the electric field $\vec{E}$ being given by

$$\vec{E} = -\dot{\vec{U}} + \nabla(\nabla\cdot\vec{U}), \tag{2}$$

and the polarization $\vec{P}$ by

$$\vec{P}(r) = \sum_{\vec{l}} \vec{P}_{\vec{l}}\,\delta(\vec{r}-\vec{l}). \tag{3}$$

The incident field is taken to be polarized in the x direction, with angular frequency ω, and direction of propagation in the y-z plane, making an angle θ with the z axis. This is the case of so-called s polarization. It is normalized so that the amplitude of the Hertz vector is unity

$$\vec{U}_{in} = \hat{x}e^{-i\omega t}e^{i(sz+qy)}, \tag{4}$$

with $\hat{x}$ denoting a unit vector in the x direction and

$$s=\omega\cos\theta, \quad q=\omega\sin\theta.$$

This system possesses a translational symmetry group in the x-y plane, consisting of all translations through integer intervals in the x and y directions and combinations of these. The solution therefore must belong to an irreducible representation of this group, and that representation is determined by the translational symmetry of the incoming wave. Accordingly, we have

$$\vec{P}_{\vec{l}} = \hat{x}\,P_n e^{-i\omega t}e^{iql_y}, \tag{5}$$

where $n=1,2,3,\ldots$ is the z component of $\vec{l}$. For the field we have

$$\vec{U}(\vec{r}) = \hat{x}e^{-i\omega t}e^{iqy}\sum_{\vec{\kappa}} u_{\vec{\kappa}}(z)e^{i\vec{\kappa}\cdot\vec{\rho}}, \tag{6}$$

where $\vec{\rho}$ is the projection of $\vec{r}$ in the x-y plane, and the summation goes over all vectors $\vec{\kappa}$ belonging to the reciprocal lattice in the x-y plane, that is, all two-dimensional vectors whose x and y components are integer multiples of 2π. Inserting (3), (5), and (6) into (1), we obtain for the coefficient $u_{\vec{\kappa}}(z)$

$$-u_{\vec{\kappa}}'' + [(q+k)^2 - \omega^2]u_{\vec{\kappa}} = 4\pi\sum_{n=1}^{\infty} P_n\delta(z-n), \tag{7}$$

where

$$(q+\kappa)^2 \equiv \kappa_x^2 + (q+\kappa_y)^2.$$

The nature of the solution to (7) depends on whether the quantity $[(q+\kappa)^2-\omega^2]$ is positive or negative. If

$$\omega^2\cos^2\theta + 4\pi\omega\sin\theta < 4\pi^2,$$

it will be negative only for $\vec{\kappa}=0$. We will assume that this is the case, but it will be clear that this is not an essential restriction. With this assumption, the retarded solution of (7) for $\vec{\kappa}=0$ is

$$u_0(z) = \frac{2\pi i}{s}\sum_n P_n e^{is|z-n|}. \tag{8}$$

For all other $\vec{\kappa}$, the solution which is well behaved at infinity is

$$u_{\vec{\kappa}}(z) = \frac{2\pi}{\gamma(\vec{\kappa})}\sum_n P_n e^{-\gamma(\vec{\kappa})|z-n|}, \tag{9}$$

where

$$\gamma^2(\kappa) = (q+\kappa)^2 - \omega^2. \tag{10}$$

To find the electric field, we use (2), (4), (6), (8),

and (9) to obtain

$$\vec{E}(\vec{r}) = \hat{x} e^{-i\omega t} e^{iqy} \left(\epsilon_{in}(z) + \epsilon_0(z) + \sum_{\vec{k}} \epsilon_{\vec{k}}(z) e^{i\vec{k}\cdot\vec{\rho}} \right), \tag{11}$$

where the sum goes over all nonzero values of $\vec{\kappa}$, and

$$\epsilon_{in}(z) = \omega^2 e^{isz}; \tag{12}$$

$$\epsilon_0(z) = \frac{2\pi i \omega^2}{s} \sum_n P_n e^{is|z-n|}; \tag{13}$$

$$\epsilon_{\vec{k}}(z) = \frac{2\pi(\omega^2 - \kappa_x^2)}{\gamma(\vec{\kappa})} \sum_n P_n e^{\gamma(\vec{k})|z-n|}. \tag{14}$$

These results are equivalent, of course, to what one would obtain by applying the methods of Nijboer, de Wette, and Schacher[13,14] to our problem.

Up to now, we have taken it for granted that all the vectors $\vec{P}$ and $\vec{U}$ are in the x direction. From (2), (6), (9), and (10), we now see that this assumption is self-consistent: the contributions to both other components from reciprocal lattice vectors differing in the sign of κ_x cancel.

We will now use Eqs. (11)–(14) for integer z to get the fields acting on the dipoles making up the crystal. As we shall see, this leads to a soluble equation for P_n. The contribution of $n=z$, however, requires special attention. This is the field exerted on a dipole in the plane at z by other dipoles in the same plane. We see that the contribution of (13) to this is finite and pure imaginary. It includes the self-damping term for the dipole, plus the out-of-phase component of the field due to the other dipoles in the same plane. The contribution of (14) is real, but diverges when summed over $\vec{\kappa}$. The reason for this is that it contains the infinite self-force due to the interaction of the dipole with its own field. This must be subtracted off, but it is inconvenient to do so in this representation. Instead, we evaluate separately the real part of the field seen by each dipole due to *other* dipoles in the same plane, and use (14) only for the contributions of other planes. The real part of the field felt by a dipole in the nth plane due to other dipoles in the same plane is easily seen from (1) and (2) to be

$$\vec{E}(\vec{l}) = P_n e^{-i\omega t} e^{iql_y} \bar{\epsilon}(\omega, q),$$

with

$$\bar{\epsilon}(\omega, q) = \mathrm{Re} \sum{}' e^{iqy} \left(\omega^2 + \frac{\partial^2}{\partial x^2} \right) \frac{e^{i\omega r}}{r}, \tag{15}$$

where the sum goes over all lattice points in the x-y plane except the origin. The function $\bar{\epsilon}(\omega, q)$ can be evaluated by techniques similar to those of Refs. 13 and 14. We have done this for a few representative values of ω and q, and the results are summarized in Table I.

TABLE I. The function $\bar{\epsilon}(\omega, q)$ defined in Eq. (15) for various values of its arguments ($q = \omega \sin\theta$).

$\sin\theta$ \ $\omega/2\pi$	0.0	0.2	0.4	0.6	0.8
0.00	4.517	0.079	−10.904	−19.826	−0.823
0.06	...	0.080	−10.885	−19.664	1.354
0.12	...	0.085	−10.829	−19.172	9.150
0.18	...	0.092	−10.735	−18.338	29.801
0.24	...	0.103	−10.604	−17.057	167.988

The equation of motion for the dipole at site $\vec{l}$ is

$$\ddot{\vec{P}}_{\vec{l}} = -\omega^2 \vec{P}_{\vec{l}} = g^2 \vec{E}(\vec{l}) - \nu^2 \vec{P}_{\vec{l}}, \tag{16}$$

where g is a coupling constant, and ν is the natural frequency of the oscillator. Using Eqs. (5) and (11)–(16) we obtain

$$\eta P_n = -\omega^2 e^{isn} + \frac{2\pi i \omega^2}{s} \sum_{n'=1}^{\infty} P_{n'} e^{is|n-n'|} + \sum_{\vec{k}\neq 0} \sum_{\substack{n'\neq n \\ n'=1}}^{\infty} \frac{2\pi(\omega^2 - \kappa_x^2)}{\gamma(\vec{\kappa})} e^{-\gamma(\vec{k})|n-n'|} P_{n'}, \tag{17}$$

where

$$\eta = g^{-2}[\nu^2 - \omega^2 - g^2 \bar{\epsilon}(\omega, q)]. \tag{18}$$

In Sec. III, we solve Eq (17) formally for P_n.

III. SOLUTION

A. The function $S(w)$

We seek a solution of (17) such that P_n does not become infinite in the limit of large n, and on physical grounds it is clear that such a solution exists. Now let w be a complex number, and define

$$S(w) = w^{-1} \sum_{n=1}^{\infty} P_n w^n. \tag{19}$$

From the above-mentioned property of P_n, it is evident that (19) defines a function analytic inside the unit circle (and perhaps inside a larger circle). Elsewhere, $S(w)$ may be defined by analytic continuation.

It is clear that a knowledge of $S(w)$ is tantamount to a complete solution of the problem. For example, we clearly have

$$P_n = \frac{1}{2\pi i} \oint \frac{S(w)\,dw}{w^n} = \frac{1}{2\pi} \int_0^{2\pi} S(e^{i\phi}) e^{-i(n-1)\phi} d\phi, \tag{20}$$

where the contour is the unit circle, or if $S(w)$ possesses poles on the unit circle, a circle with radius very slightly less than unity. Having eval-

uated P_n from (20), the field at any point can be evaluated using Eqs. (11)–(14). In particular, the reflection coefficient, which is essentially the amplitude u_0 for negative z, is easily seen, with the aid of (8), to be

$$R = \frac{2\pi i}{s} e^{is} S(e^{is}). \tag{21}$$

To get a little further insight into $S(w)$, consider the case where there is a solution expressible in terms of a finite or infinite number of refractive indices

$$P_n = \sum_j p_j e^{i\kappa_j n}, \tag{22}$$

with refractive indices

$$n_j = \omega^{-1}(\kappa_j^2 + q^2)^{1/2}.$$

If P_n is given by (22), then we immediately find for $S(w)$

$$S(w) = \sum_j \frac{p_j}{e^{-i\kappa_j} - w}. \tag{23}$$

Thus, the "refractive indices" are essentially determined by the poles of $S(w)$.

In the next subsection, we recast (17) into an equation for $S(w)$, and solve it formally.

B. Formal evaluation

We note that there can be more than one $\vec{\kappa}$ in (17), with the same value of $\gamma(\vec{\kappa})$. It can clearly be written in the form

$$\eta P_n = \omega^2 e^{isn} + i\lambda_0 \sum_{n'=1}^{\infty} P_{n'} e^{is|n-n'|} + \sum_\alpha \lambda_\alpha \sum_{\substack{n'=1 \\ n' \neq n}}^{\infty} e^{-\gamma_\alpha |n-n'|}, \tag{24}$$

where now all the γ_α are different, and the coefficients $\lambda_0, \lambda_\alpha$, are, of course, defined in such a way that (24) is equivalent to (17).

We now multiply both sides of (24) by w^{n-1}, (with $|w| < 1$) and sum over n, obtaining

$$\eta S(w) = \frac{\omega^2}{e^{-is} - w} + i\lambda_0 Q_0 + \sum_\alpha \lambda_\alpha Q_\alpha, \tag{25}$$

where

$$\begin{aligned} Q_0 &= w^{-1} \sum_{n,n'=1}^{\infty} w^n P_{n'} e^{is|n-n'|} \\ &= w^{-1} \sum_{n'=1}^{\infty} P_{n'} \left(e^{isn'} \sum_{n=1}^{n'-1} w^n e^{-isn} + e^{-isn'} \sum_{n=n'}^{\infty} w^n e^{isn} \right) \\ &= w^{-1} \sum_{n'=1}^{\infty} P_{n'} \left[e^{isn'} \left(\frac{we^{-is} - w^{n'} e^{-isn'}}{1 - we^{-is}} \right) + \frac{w^{n'}}{1 - we^{is}} \right] \\ &= \frac{e^{is} S(e^{is})}{e^{is} - w} + \left(\frac{2i \sin s}{w + w^{-1} - 2\cos s} \right) S(w), \end{aligned} \tag{26}$$

and similarly

$$\begin{aligned} Q_\alpha &= w^{-1} \sum_{\substack{n'=1 \\ n' \neq n}}^{\infty} w^n P_{n'} e^{-\gamma_\alpha |n-n'|} \\ &= \frac{e^{-\gamma_\alpha} S(e^{-\gamma_\alpha})}{e^{-\gamma_\alpha} - w} - S(w) \left(\frac{w + w^{-1} - 2e^{-\gamma_\alpha}}{w + w^{-1} - 2\cosh\gamma_\alpha} \right). \end{aligned} \tag{27}$$

Equations (25)–(27), with some rearrangement, can be written as

$$\mathcal{F}(w) S(w) = \mathcal{G}(w), \tag{28}$$

with

$$\mathcal{F}(w) = \eta + \frac{2\lambda_0 \sin s}{w + w^{-1} - 2\cos s} + \sum_\alpha \lambda_\alpha \frac{w + w^{-1} - 2e^{-\gamma_\alpha}}{w + w^{-1} - 2\cosh\gamma_\alpha}, \tag{29}$$

$$\mathcal{G}(w) = \frac{\omega^2}{e^{-is} - w} + \frac{i\lambda_0 S(e^{is}) e^{is}}{e^{is} - w} + \sum_\alpha \frac{\lambda_\alpha e^{-\gamma_\alpha} S(e^{-\gamma_\alpha})}{e^{-\gamma_\alpha} - w}. \tag{30}$$

Temporarily, for bookkeeping purposes, we assume that the sum over α in (29) and (30) is cut off after N terms. The passage to the limit $N \to \infty$ will cause no difficulty. With this proviso, we see that the function $\mathcal{F}(w)$ has $2(N+1)$ poles, located at

$$y_0, y_0^{-1}; y_\alpha, y_\alpha^{-1} \quad (\alpha = 1, 2, \ldots, N),$$

where by definition $y_0 = e^{-is}$, $y_\alpha = e^{\gamma\alpha}$ $(\alpha = 1, 2, \ldots, N)$. Thus, the y's are all outside the unit circle, the y^{-1} inside. [Remember that s must be given a small positive imaginary part in order to carry out the summation in obtaining (25).] For convenience, we assume that the index α has been arranged in order of increasing γ_α.

$\mathcal{F}(w)$ is also seen to have $2(N+1)$ zeros, also in reciprocal pairs, which we again order according to increasing absolute value of the larger members of the pairs, and call

$$x_0, x_0^{-1}, x_\alpha, x_\alpha^{-1}.$$

Again, the convention is that the x's are outside the unit circle, the x^{-1} inside.

The function $\mathcal{G}(w)$ has poles at $y_0, y_0^{-1}, y_\alpha^{-1}$ $(\alpha = 1, 2, \ldots, N)$. It has $N+1$ zeros.

Referring to (28), and remembering that $S(w)$ is analytic inside the unit circle, we conclude that each zero of $\mathcal{F}(w)$ within the unit circle is also a zero of $\mathcal{G}(w)$. However, since $\mathcal{F}(w)$ has $(N+1)$ such zeros, and the total number of zeros of $\mathcal{G}(w)$ is also $(N+1)$, we conclude that these are the *only* zeros of $\mathcal{G}(w)$. We also see from (29) and (30) that both $\mathcal{F}$ and $\mathcal{G}$ are rational functions, with $\mathcal{G}$ falling off as w^{-1} for large w, while $\mathcal{F}$ approaches a finite limit. Accordingly, the two functions can

be written as

$$\mathcal{G}(w) = \frac{G_0}{w - y_0} \prod_{\alpha=0}^{N} \frac{w - x_\alpha^{-1}}{w - y_\alpha^{-1}}; \tag{31}$$

$$\mathcal{F}(w) = F_0 \prod_{\alpha=0}^{N} \frac{(w - x_\alpha)(w - x_\alpha^{-1})}{(w - y_\alpha)(w - y_\alpha^{-1})}, \tag{32}$$

where G_0 and F_0 are constants. From (28), (31), (32), we obtain for $S(w)$

$$S(w) = \frac{S_0}{w - y_0} \prod_{\alpha=0}^{N} \frac{w - y_\alpha}{w - x_\alpha} = \frac{S_0}{w - x_0} \prod_{\alpha=1}^{N} \frac{w - y_\alpha}{w - x_\alpha}, \tag{33}$$

where $S_0 = G_0/F_0$. Equation (33) gives $S(w)$ in terms of the zeros and poles of $\mathcal{F}(w)$, if we can determine the constant S_0. This is easily done by noting that, according to (30), the residue of $\mathcal{G}$ at $w = y_0$ is $-w^2$, while according to (28), it is the residue of $\mathcal{F}$ at the same point multiplied by $S(y_0)$. Setting these two equal, it is a simple matter to obtain

$$S_0 = \frac{is}{2\pi y_0} (y_0 - x_0) \prod_{\alpha=1}^{N} \frac{y_0 - x_\alpha}{y_0 - y_\alpha},$$

and

$$S(w) = \frac{is}{2\pi y_0} \left(\frac{y_0 - x_0}{w - x_0}\right) \prod_{\alpha=1}^{N} \frac{(y_0 - x_\alpha)(w - y_\alpha)}{(y_0 - y_\alpha)(w - x_\alpha)}. \tag{34}$$

Equation (34) gives the function $S(w)$ in terms of the poles and zeros of $\mathcal{F}(w)$. For $N = 1$, it is the same as Eq. (57) of Ref. 7, where, however, the definition of the function $\tilde{R}$ differs from our S by a multiplicative constant, and only normal incidence is considered. The passage to the limit $N \to \infty$ in (34) causes no difficulties, as the infinite product clearly converges. If desired, the poles of S (zeros of $\mathcal{F}$ outside the unit circle) may be interpreted in terms of refractive indices with the aid of (23). One sees that our function $\mathcal{F}(w)$ is an obvious generalization of the function whose zeros determined the refractive indices in Ref. 7 for the case $N = 1$.

Our task is not yet complete, however, since direct use of (34) requires a knowledge of the location of all the zeros of $\mathcal{F}$, and the task of finding these becomes prohibitively laborious as N becomes large. In Sec. III C, we see how we can bypass the problem of finding the roots of $\mathcal{F}(w) = 0$.

C. Bypassing the roots

Define the function

$$\begin{aligned}\overline{\mathcal{F}}(w) &= \lambda_0 \sin s + \tfrac{1}{2}(w + w^{-1} - 2\cos s) \\ &\quad \times \left[\eta + \sum_{\alpha=1}^{N} \lambda_\alpha \left(\frac{w + w^{-1} - 2e^{-\gamma_\alpha}}{w + w^{-1} - 2\cosh\gamma_\alpha}\right)\right] \\ &= \frac{1}{2w}(w - y_0)(w - y_0^{-1})\mathcal{F}(w) \\ &= \frac{F_0}{2w}(w - x)(w - x_0^{-1}) \prod_{\alpha=1}^{N} \frac{(w - x_\alpha)(w - x_\alpha^{-1})}{(w - y_\alpha)(w - y_\alpha^{-1})},\end{aligned} \tag{35}$$

with

$$\ln\mathcal{F}(w) = \ln\left(\frac{F_0}{2}\right) + \ln\frac{w - x_0^{-1}}{w} + \sum_{\alpha} \ln\frac{w - x_\alpha^{-1}}{w - y_\alpha^{-1}} + \ln\left((w - x_0)\prod_{\alpha=1}^{N}\frac{w - x_\alpha}{w - y_\alpha}\right). \tag{36}$$

We now make use of the easily verifiable result

$$\oint \ln\left(\frac{\zeta - a}{\zeta - b}\right)\frac{d\zeta}{\zeta - w} = 0, \tag{37}$$

if the contour encloses all three points a, b, w. Using (36) and (37), we find

$$\frac{1}{2\pi i}\oint \ln\overline{\mathcal{F}}(s)\frac{d\zeta}{\zeta - w} = \ln\left(\frac{F_0}{2}(w - x_0)\prod_{\alpha=1}^{N}\frac{w - x_\alpha}{w - y_\alpha}\right), \tag{38}$$

where the contour is the unit circle, either raised or lowered slightly in the imaginary direction according as $\sin s$ is positive or negative (so as to enclose x_0^{-1} but not x_0, if these are on the unit circle), plus a small circle about w if w is not already contained in the original contour. The result follows from the fact that the contributions of the poles and zeros inside the contour are all zero by (37), leaving just the ones outside. Note that one can always pair off zeros and poles and run a branch line from each zero to its associated pole in such a way that none of these branch lines cross the contour of integration. Comparing (38) with (34), we see immediately that

$$\begin{aligned}\ln\left(\frac{2\pi y_0}{is}S(w)\right) &= \frac{1}{2\pi i}\oint \ln\overline{\mathcal{F}}(s)\left(\frac{1}{\zeta - y_0} - \frac{1}{\zeta - w}\right)d\zeta \\ &= \frac{1}{2\pi i}\oint \ln\overline{\mathcal{F}}(s)\frac{y_0 - w}{(\zeta - y_0)(\zeta - w)}d\zeta,\end{aligned} \tag{39}$$

where the contour now also encloses y_0. Equation (39), together with (35), is the promised "formally closed" solution. To use it, one must sum the series (35) to obtain the function $\overline{\mathcal{F}}(w)$, and then perform the contour integration defined by (39). Unlike the situation with the Mahan-Obermair or exp methods, one can do both of these steps as accurately as one wishes without great increase in computational effort.

D. The reflection coefficient

The case of greatest practical interest is that of the reflection coefficient R, which, according to (21) and (39) is given by

$$R = -e^{2is}e^{U}, \tag{40}$$

with

$$U=\frac{1}{2\pi i}\oint \ln\mathfrak{F}(\zeta)\left(\frac{1}{\zeta-e^{-is}}-\frac{1}{\zeta-e^{is}}\right)d\zeta. \quad (41)$$

We note that $\mathfrak{F}(\zeta)$ is really a function only of $\cos\phi = \frac{1}{2}(\zeta+\zeta^{-1})$. In the Mahan-Obermair approach, this function is approximated by a polynomial, which we can take to be written in factored form

$$\mathfrak{F}(s)=K\prod_j(\zeta+\zeta^{-1}-x_j-x_j^{-1}), \quad (42)$$

where x_j has absolute value greater than unity or, if the absolute value is equal to unity, has an imaginary part with the same sign as that of e^{-is}. The logarithm is given by

$$\ln\mathfrak{F}(s)=\ln K+\sum_j \ln\frac{(\zeta-x_\alpha^{-1})(\zeta-x_\alpha)}{\zeta}. \quad (43)$$

We now insert (43) into (40), (41), use (37), and note that the contour includes the x^{-1} but not the x's themselves. The result is easily seen to be

$$R=-e^{2is}\prod_j\left(\frac{e^{-is}-x_j}{e^{is}-x_j}\right), \quad (44)$$

which is also the Mahan-Obermair result. It is quite easy to verify that one also recovers the exp model result by keeping only one term in the sum over α in (29).

Returning to the exact expression (41), we see that the integrand has two types of singularities on the unit circle: poles at $\zeta=e^{is}$ and e^{-is}, and logarithmic singularities at the zeros, if any, of $\mathfrak{F}(s)$ on the unit circle. Such zeros clearly always appear in complex conjugate (reciprocal) pairs. There can never be more than three such pairs, and the author does not know of any actual cases where there are more than two. In any case, it is convenient, though not absolutely necessary, to separate out the contributions of the various singularities. Accordingly, let $\xi=\cos\phi=\frac{1}{2}(\zeta+\zeta^{-1})$, and let the zeros of $\mathfrak{F}(\zeta)$ for $-1\le\xi\le1$ be at $\xi=\cos\sigma_j$, with j taking on at most three values. We then write

$$\mathfrak{F}(\zeta)=\mathfrak{F}(\cos s)\Phi(\xi)\prod_j\left(\frac{\xi-\cos\sigma_j}{\cos s-\cos\sigma_j}\right). \quad (45)$$

Taking the logarithm of (45) and inserting it into (41), we see that $\ln\mathfrak{F}(\cos s)$ and $\ln(\cos s-\cos\sigma_j)$

TABLE II. The reflection coefficient R, for $\omega/2\pi=0.8$, $\sin\theta=0.24$, as a function of $\bar{\eta}=|s/2\pi\omega^2\sin s|\eta$, calculated by various methods, viz: (a) Exactly using Eq. (47). (b) With the exp. model, replacing the sum in Eq. (29) by the single term with the smallest value of γ. In this case, this was the term with $\kappa_x=0$, $\kappa_y=-2\pi$, $\gamma=0.7126$. (c) With the Mahan-Obermair method, $N=1$. Range for which $|R|=1$: (a) $-5.33<\bar{\eta}<3.06$, (b) $-5.36<\bar{\eta}<3.09$, (c) $-4.07<\bar{\eta}<6.33$.

	(Re R)$\times 10^2$			(Im R)$\times 10^2$		
$\bar{\eta}$	*a*	*b*	*c*	*a*	*b*	*c*
−10	−4.706	−4.738	−3.838	4.921	4.889	2.947
−9	−5.922	−5.964	−4.656	5.305	5.258	2.705
−8	−7.800	−7.860	−5.821	5.617	5.540	1.733
−7	−11.05	−11.14	−4.715	5.493	5.337	-9.666×10^{-9}
−6	−18.05	−18.23	−4.135	2.550	1.993	-8.476×10^{-9}
−5	−88.62	−86.62	−3.857	46.33	49.98	3.067×10^{-8}
−4	−13.23	−12.28	−94.28	99.12	99.24	33.33
−3	40.75	41.11	−26.63	91.32	91.16	96.39
−2	76.16	76.25	24.68	64.80	64.70	96.91
−1	95.55	95.54	61.99	29.49	29.54	78.47
0	99.51	99.54	86.49	−9.838	−9.616	50.20
1	86.84	87.05	98.61	−49.58	−49.21	16.60
2	52.83	53.53	98.15	−84.90	−84.47	−19.15
3	−32.04	−27.76	84.20	−94.73	−96.07	−53.95
4	−1.873	−1.880	54.88	−2.755	−2.739	−83.60
5	−1.790	−1.796	− 6.624	−2.631	−2.631	−99.78
6	−1.721	−1.726	−67.92	−2.528	−2.515	−73.40
7	−1.664	−1.669	−5.547	−2.443	−2.431	-2.701×10^{-8}
8	−1.618	−1.622	−9.292	−2.374	−2.363	−1.445
9	−1.581	−1.585	−6.045	−2.319	−2.309	−4.757
10	−1.555	−1.557	−4.275	−2.279	−2.269	−4.986

contribute nothing to the integral, while the other factors involving the σ_j contribute a factor similar to (44). We thus have for R

$$R = -e^{2is}[\exp(\Gamma)] \prod_j \left(\frac{e^{-is} - e^{-i\sigma_j}}{e^{is} - e^{-i\sigma_j}} \right) , \tag{46}$$

with

$$\Gamma = \frac{1}{2\pi i} \oint \ln\Phi \left(\frac{1}{\zeta - e^{-is}} - \frac{1}{\zeta - e^{is}} \right) d\zeta$$

$$= -\frac{i \sin s}{\pi} \int_0^\pi \frac{\ln\Phi(\cos\phi) d\phi}{\cos\phi - \cos s} . \tag{47}$$

The function Φ is positive everywhere in the range of integration, and its logarithm is zero at $\cos\phi = \cos s$, so the integrand in (47) possesses no singularities, and the integral is easily evaluated by numerical means. Equations (46) and (47) appear to afford the best basis for practical calculations of the reflection coefficient.

In Table II, we show some results for the reflection coefficient, calculated as a function of η, for $\omega/2\pi = 0.8, \sin\theta = 0.24$. (Of course, if g is small, η can vary over a wide range with only negligible change in ω). For comparison, results of the exp model, and of the Mahan-Obermair method with $N = 1$, are also listed. In this case, the error committed by using the exp model is not great, while that incurred with the Mahan-Obermair method is considerable. This is not always true, however. This case was deliberately chosen to be a particularly bad one for the Mahan-Obermair method, and one could equally well choose cases where the exp model fails badly and the Mahan-Obermair approach does well.

IV. DISCUSSION

It is hoped that the approach developed here will provide a useful basis for practical calculations, as well as providing theoretical insight. For theoretical purposes, the study of the analytic structure of the function $S(w)$ would appear to provide a fruitful field, while practical calculations using (46) and (47) are quite easy to do with as much accuracy as one wishes. The main defect at this point is the limitation to s polarization. The author hopes to remove this limitation in a future article.

It is perhaps worthwhile to say something about the limits of validity of the Mahan-Obermair and exp models. The Mahan-Obermair approach with small N is a good approximation if the falloff of the interaction is sufficiently fast, i.e., if all the $\gamma(\vec{\kappa})$ defined by Eq. (10) are sufficiently large. It will fail completely if one or more of them is small. The smallest γ is evidently obtained for $\kappa_y = -2\pi$, $\kappa_x = 0$, for which

$$\gamma^2 = 4\pi^2 - \omega^2 \cos^2\theta - 4\pi\omega \sin\theta. \tag{48}$$

If $\omega > \pi$, this can be made as small as one wishes, even negative. Just such a case was deliberately chosen in arriving at the results shown in Table II.

As for the exp model, it will be at its best if one of the γ is much smaller than the others. It will fail badly if the two smallest γ's are nearly, but not quite, equal, as will always be the case for small, but nonvanishing, angle of incidence.

The Mahan-Obermair method is completely inappropriate for studying the analytic structure of the function $S(w)$ since, as shown in Ref. 7, nearly all its poles for large N are clustered around the circle with radius e^{γ_0}, where γ_0 is the smallest of the γ's defined by Eq. (10), and bear no relation to poles of the exact $S(w)$. This fact, however, has little bearing on the practical utility of the Mahan-Obermair method. The $N+1$ poles given by the exp method with N exponentials included, on the other hand, are located close to $(N+1)$ of the infinite number of actual poles of $S(w)$.

Finally, there is the question of what happens if some of the γ^2 defined by Eq. (10) are negative. The answer is quite simple: one simply handles these terms in the same way as the term with $\vec{\kappa} = 0$, obtaining solutions similar to (8) instead of (9). There will then be more than one reflected wave, corresponding to the usual diffraction situation.

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