SCATTERING BY STRIPE GRATING

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Abstract. We consider the scattering problem of $e^{i\vec{q}\cdot\vec{r}}$ by a slab S with L–periodic potential in the x direction, $V = \pm V_0$ on each half–period (V_0 constant). It is proved that there exists a unique solution. We also derive the asymptotic behavior of the solution away from the slab.

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§1. Introduction. We denote a variable point in $\mathbb{R}^3$ by $X = (x_1, x_2, x_3)$, $X = (x, y, z)$ or $\vec{r}$. We shall consider the scattering of a beam of particles incident to a slab S from below. S has a thickness d and is given by $\left\{ |z| < \frac{d}{2} \right\}$. The potential V of the slab is independent of y and, as a function of x, is given by

$$V(x) = \begin{cases} V_0 & \text{if} \quad 0 < x < \frac{L}{2} \\ -V_0 & \text{if} \quad \frac{L}{2} < x < L\,, \end{cases} \tag{1.1}$$
$$V(x + mL) = V(x) \quad \text{for} \quad m = \pm 1, \pm 2, \ldots$$

Thus, the potential $V(X)$ in the entire space is given by

$$V(x, y, z) = \begin{cases} V(x) & \text{if} \quad |z| < \frac{d}{2} \\ 0 & \text{if} \quad |z| > \frac{d}{2}\,. \end{cases} \tag{1.2}$$

The Schrödinger equation for the wave function Ψ is

$$i\frac{\partial \Psi}{\partial t} + \Delta \Psi - V\Psi = 0 \tag{1.3}$$

where V is defined by (1.2). A beam of particles of energy E and wave vector $\vec{q} = (q_1, q_2, q_3)$ $\quad (|\vec{q}|^2 = E)$ is represented in free space by

$$e^{i\vec{q}\cdot r}\, e^{-iEt}\,.$$

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We try to find a solution of (1.3) of the form

$$\Phi(\vec{r})e^{-iEt} .$$

It follows that

$$\Delta\Phi + E\Phi = V\Phi . \tag{1.4}$$

Introducing Green's function of $\Delta + E$ in $\mathbf{R}^3$

$$-\frac{1}{4\pi} \frac{e^{i|\vec{q}|\,|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} ,$$

we formally conclude that Φ is a solution of (1.4) if and only if

$$\Phi(\vec{r}) = e^{i\vec{q}\cdot\vec{r}} - \frac{1}{4\pi} \int_{\mathbf{R}^3} \frac{e^{i|\vec{q}|\,|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} V(\vec{r}\,')\Phi(\vec{r}\,')\, d^3r' ; \tag{1.5}$$

this is the Lippmann–Schwinger equation. For more details on the physical background we refer to Gottfried [7; Section 12].

The equation

$$\Phi(\vec{r}) = \Phi_0(\vec{r}) - \frac{1}{4\pi} \int_{\mathbf{R}^3} \frac{e^{i|\vec{q}|\,|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} V(\vec{r}\,')\Phi(\vec{r}\,')\, d^3r' \tag{1.6}$$

was studied by Ikebe [9] under the assumption that $V(X)$ is Hölder continuous in $\mathbf{R}^3$ (except for a finite number of L^2 singularities) and

$$|V(X)| \leq \frac{C}{|X|^{2+\epsilon}} \qquad \text{for} \qquad |X| > \mathbf{R}_0 \tag{1.7}$$

where C, R_0, ϵ are some positive constants. Denote by B the set of all functions in $C^0(\mathbf{R}^3) \cap L^\infty(\mathbf{R}^3)$ which vanish at ∞. Ikebe proved that the Riesz–Schauder–Fredholm alternative is valid for (1.6) in the space B. He then used this result to develop the spectral theory for the Schrödinger operator $-\Delta + V$ in $\mathbf{R}^3$ and to establish existence and properties of the wave operators $W_\pm$ and of the S matrix. More recently Agmon [1] has established, by an entirely different method, the same results concerning the spectral theory and $W_\pm, S$ for much more general elliptic operators, including, in particular, $-\Delta + V$ with

$$|V(X)| \leq \frac{C}{(1 + |X|)^{1+\epsilon}} \tag{1.8}$$

for some $C > 0$, $\epsilon > 0$; potentials satisfying (1.8) are referred to as ***short range potentials***. These results can be extended to potentials $V + V_1$ where V is short range and $V_1 = V_1(|X|)$ is a radial function which need not even be bounded at ∞; see Ben–Artzi [2]. For further work by other authors on both short range potentials and long range radial potentials see the references in [1] [2] [9].

The potential (1.1), (1.2) used in this paper does not satisfy the short range condition and, of course, it is not radial. Thus it is not included in the class of potentials for which scattering theory has been developed. The interest in this particular potential comes from industry:*

If one substitutes bismuth at certain lattice points of rare earth garnet crystals, one gets a material which exhibits an almost ideal magnetic stripe domain structure. The structure consists of a one–dimensional periodic array of regions of nearly constants magnetization, so that the magnitudes of magnetization vectors in two adjacent regions are the same, but their directions are opposite. This condition produces the alternating–sign magnetic permeability tensors. When a beam of light is passed through such a film, it splits into many diffracted beams. The angles of the diffracted–beam directions relative to the incident–beam direction are determined by the periodicity length.

By appropriate tuning of the material parameters and film thickness one can achieve high–efficiency beam deflection. That is, it is possible to channel most of the incident energy into a single beam which is at a specific angle to the incident beam.

It is an important property at these garnet films that the application of a magnetic field can modify the stripe domain structure. It is possible in this way to rotate the direction of periodicity and to change the periodicity length. Thus, one has the ability to vary both the azimuthal and the polar deflection angles purely electronically (i.e., without mechanically modifying the grating).

Here we consider the mathematically simpler case of diffraction of particles by a stripe grating of a potential field V (rather than a magnetic one). Thus instead of working with the vector potential (Coulomb gauge) and a matrix V, we work with the single scalar equation (1.4).

Robert Ore [11] has recently examined the effect of the stripe grating on the beam $e^{i\vec{q}\cdot\vec{r}}$. He used the method of superposition of solutions both inside the slab and outside it and, by means of consistency conditions along the boundary of the slab, obtained a formal expansion

$$\Phi(X) = \begin{cases} e^{i\vec{q}\cdot X} + \sum\limits_{n=-\infty}^{\infty} T_n \, e^{i\vec{q}_n^{\,+}\cdot X} & \text{if} \quad z > \frac{d}{2} \\ e^{i\vec{q}\cdot X} + \sum\limits_{n=-\infty}^{\infty} R_n \, e^{i\vec{q}_n^{\,-}\cdot X} & \text{if} \quad z < -\frac{d}{2} \end{cases} . \tag{1.9}$$

*We wish to thank Dr. Robert Ore from UNISYS (Minneapolis, Minn.) for introducing us to this problem and for many useful conversations.

Here $\vec{q}_n^{\pm}$ are defined by

$$(1.10) \qquad \left(q_1 + \frac{2\pi n}{L}, q_2, \pm\left[|\vec{q}^{\,2}| - \left(q_1 + \frac{2\pi n}{L}\right)^2 - q_2^2\right]^{1/2}\right), \quad q = |\vec{q}|$$
$$\text{where} \quad n = 0, \pm 1, \pm 2, \ldots$$

and the *transmission coefficients* T_n and *reflection coefficients* R_n are determined by solving appropriate transcendental equations. Notice that only a finite number of the third component of $\vec{q}_n^{\pm}$ are real; the imaginary ones give rise to exponentially decaying terms in (1.9), as $|z| \to \infty$. Ore was able to solve numerically the first few coefficients. Another approach (see, e.g., Cowley [3; Chap. 10]) is to assume that all the R_n, T_n vanish if $|n| > N$ and compute $R_0, R_{\pm 1}, T_0, T_{\pm 1}, \ldots, R_{\pm N}, T_{\pm N}$.

In this paper we shall study (rigorously) equation (1.6) when Φ_0 has the form

$$(1.11) \qquad \Phi_0(X) = e^{i\vec{q}\cdot X} f(x_1, x_3), \qquad f(x_1, x_3) \ \text{bounded and periodic in } x_1 \text{ of period } L$$

($f \equiv 1$ corresponds to (1.5)), and seek a solution Φ of the form

$$(1.12) \qquad \Phi(X) = e^{i\vec{q}\cdot X} \phi(x_1, x_3), \quad \phi(x_1, x_3) \ \text{bounded and periodic in } x_1 \text{ of period } L.$$

Then (1.6) reduces to

$$(1.13) \qquad \phi(x_1, x_3) = f(x_1, x_3) - \frac{V_0}{4\pi} \int_{\mathbf{R}^3} \frac{e^{-i\vec{q}\cdot(X-Y)} e^{iq|X-Y|}}{|X-Y|} \widetilde{V}(Y) \phi(y_1, y_3)\, dY$$

where $V(Y) = V_0 \widetilde{V}(Y)$, or, briefly,

$$(1.14) \qquad \phi = f + V_0 K \phi$$

where

$$(1.15) \qquad (Kg)(x_1, x_3) = \frac{1}{4\pi} \int_{\mathbf{R}^3} \frac{e^{-i\vec{q}(X-Y)} e^{iq|X-Y|}}{|X-Y|} \widetilde{V}(Y) g(y_1, y_2)\, dY.$$

In particular, equation (1.5) reduces to

$$(1.16) \qquad \phi = 1 + V_0 K \phi, \ \phi = \phi(x_1, x_2).$$

In §2 we shall compute $K1$ and in §3 we shall evaluate Kf, f as in (1.11). Next, in §4 we prove that K is a bounded compact operator in the space

$$B = \{\phi(x_1, x_3),\ \phi \text{ is bounded and periodic in } x_1 \text{ of period } L\}$$

with norm

$$\|\phi\| = \sup_{x_3 \in \mathbf{R}} \int_0^L |\phi(x_1, x_3)|^2 \, dx_1 .$$

By the Fredholm alternative it then follows that there is a countable set of positive numbers $W_j, W_j \to \infty$, such that if $V_0 \neq W_j$ for all j then (1.14) has a unique solution ϕ in B for any f in B. Further, $e^{i\vec{q}\cdot X} K\phi$ has the expansion (1.9) and therefore, in particular, any solution of (1.5) has the expansion (1.9).

Finally, using the results of §§2,3 we shall derive an algorithm for computing the coefficients T_n, R_n in (1.9) in case the norm of K is small; more precisely, in case

$$V_0 d \leq \frac{1}{C}$$

where C is a positive constant depending only on $\vec{q}$.

§2. Computation of K1. In this section we evaluate the integral

$$(K1)(X) = -\frac{1}{4\pi} \int e^{-\vec{q}\cdot(X-Y)} \frac{e^{iq|X-Y|}}{|X-Y|} \widetilde{V}(Y) \, dY \tag{2.1}$$

where V is defined by (1.1), (1.2), $V = V_0 \widetilde{V}$ and $q = (q_1^2 + q_2^2 + q_3^2)^{1/2}$. By a change of variables $X - Y = Z$ we have

$$\begin{aligned} -(K1)(X) &= \frac{1}{4\pi} \int_{\mathbf{R}^3} e^{-i\vec{q}\cdot Z} \frac{e^{iq|Z|}}{|Z|} \widetilde{V}(X - Z) \, dZ \\ &= \frac{1}{4\pi} \int_{\{-\frac{d}{2} < x_3 - z_3 < \frac{d}{2}\}} e^{-iq_3 z_3} dz_3 \int_{\mathbf{R}^2} e^{-i(q_1 z_1 + q_2 z_2)} \frac{e^{iq|Z|}}{|Z|} \widetilde{V}(X - Z) dz_1 dz_2 . \end{aligned} \tag{2.2}$$

The inner integral can be written as

$$J_* = 2 \int_{-\infty}^{\infty} \widetilde{V}(x_1 - z_1) G(z_1, z_3) \, dz_1$$

where

$$G(z_1, z_3) = \int_0^\infty e^{-i(q_1 z_1 + q_2 z_2)} \frac{e^{iq(z_1^2 + z_2^2 + z_3^2)^{1/2}}}{(z_1^2 + z_2^2 + z_3^2)^{1/2}} \, dz_2 . \tag{2.3}$$

Recalling the definition of $V(x)$ in (1.1) we easily find that

$$J_* = -2V_0 \int_{x_1}^{x_1+L/2} \sum_{n=-\infty}^{\infty} \left[G(t+2n\frac{L}{2}\,, z_3) - G(t+(2n+1)\frac{L}{2})\,, z_3) \right] dt \tag{2.4}$$

We shall use the Poisson summation formula* (see [4; p. 52])

$$\sum_{n=-\infty}^{\infty} f(x+nb) = \frac{1}{b} \sum_{m=-\infty}^{\infty} F\left(\frac{2\pi m}{b}\right) e^{-i\frac{2\pi m x}{b}} \tag{2.5}$$

where the convergence of the series on the right–hand side is in the sense of $\lim\limits_{N\to\infty} \sum\limits_{m=-N}^{N}$ and

$$F(y) = \int_{-\infty}^{\infty} e^{iyt} f(t)\, dt\ ,$$

provided

$$\sum_{n=-\infty}^{\infty} f(x'+nb) \quad \text{is uniformly convergent for} \quad 0 \le x' \le b \quad \text{to some function} \quad k(x'), \tag{2.6}$$

and

$$\text{the Fourier series of } k(x') \quad (\Sigma a_n\, e^{inx'}) \quad \text{is convergent to } k(x') \quad \text{at} \quad x' = x. \tag{2.7}$$

LEMMA 2.1. *The function*

$$f(x) = e^{-iq_1 x} \frac{e^{iq(x^2+z_2^2+z_3^2)^{1/2}}}{(x^2+z_2^2+z_3^2)^{1/2}} \tag{2.8}$$

satisfies the conditions (2.6), (2.7) for any z_2, z_3.

Proof. We shall show that the series in (2.6) is uniformly convergent together with its derivative. Setting $A^2 = z_2^2 + z_3^2$ and taking for simplicity $b = 1$, we can write

$$\sum_{n=-\infty}^{\infty} f(x+nb) = \Sigma\, e^{-i\, q_1(x+n)} \frac{e^{iq((x+n)^2+A^2)^{1/2}}}{((x+n)^2+A^2)^{1/2}}$$

$$= \Sigma e^{-iq_1(x+n)} \frac{e^{iq(x+n)[1+O(\frac{1}{n^2})]}}{(x+n)[1+O(\frac{1}{n^2})]}$$

$$= \sum \frac{e^{i(q-q_1)(x+n)}}{x+n} + \sum \frac{e^{i(q-q_1)(x+n)}}{x+n} O\left(\frac{1}{n^2}\right) .$$

*We would like to thank Stefen Wainger for suggesting the use of this formula.

The last series is uniformly convergent together with its derivative. Writing the first series on the right–hand side in the form

$$e^{i(q-q_1)x}\,\Sigma\,\frac{e^{i(q-q_1)n}}{n} - \Sigma\,\frac{xe^{i(q-q_1)(x+n)}}{n(n+x)}$$

we see that it is also uniformly convergent together with its first derivative. Hence $\Sigma f(x+n)$ is uniformly convergent to a continuously differentiable function, $\tilde{f}$, and its Fourier series is therefore convergent everywhere to $\tilde{f}$. Thus the conditions (2.6), (2.7) hold for the function in (2.8)

Applying the Poisson summation formula to the function

$$f(t) - f(t+\frac{L}{2})$$

where f is given by (2.8) and then integrating with respect to z_2, $0 < z_2 < \infty$, we deduce (upon recalling (2.3)) that

$$\begin{aligned}&\sum_{m=-\infty}^{\infty}\left[G(t+nL,z_3) - G(t+nL+\frac{L}{2},z_3)\right]\\ &= \frac{1}{L}\int_0^\infty \sum_{m=-\infty}^{\infty} F\left(\frac{2\pi m}{L},z_2,z_3\right)\left[e^{-i\frac{2m\pi}{L}t} - e^{-i\frac{2m\pi}{L}(t+\frac{L}{2})}\right]\end{aligned} \tag{2.9}$$

where

$$\begin{aligned}F(t,z_2,z_3) &= \int_{-\infty}^{\infty} e^{i((t-q_1)y-q_2z_2)}\frac{e^{iq(y^2+z_2^2+z_3^2)^{1/2}}}{(y^2+z_2^2+z_3^2)^{1/2}}\,dy\\ &= 2\int_0^\infty \cos((t-q_1)y)e^{-iq_2z_2}\frac{e^{iq(y^2+z_2^2+z_3^2)^{1/2}}}{(y^2+z_2^2+z_3^2)^{1/2}}\,dy\,.\end{aligned}$$

Therefore

$$\begin{aligned}&\sum_{m=-\infty}^{\infty}\left[G(t+nL,z_3) - G(t+nL+\frac{L}{2},z_3)\right]\\ &= \sum_{\substack{m=-\infty\\ m\neq 0}}^{\infty} B_m(t)\int_0^\infty F\left(\frac{2\pi m}{L},z_2,z_3\right)\,dz_2, \qquad \text{where}\end{aligned} \tag{2.11}$$

$$B_m(t) = \frac{2}{L}\left[e^{i\frac{2m\pi t}{L}} - e^{-i\frac{2m\pi}{L}(t+\frac{L}{2})L}\right]\,.$$

We proceed to evaluate
(2.12)

$$H(\alpha) \equiv \int_0^\infty F(\alpha, z_2, z_3)\, dz_2 = 4 \int_0^\infty \int_0^\infty \cos((\alpha - q_1)y) \cos(q_2 z_2) \frac{e^{iq(y^2+z_2^2+z_3^2)^{12}}}{(y^2 + z_2^2 + z_3^2)^{1/2}}\, dy\, dz_2.$$

assuming first

$$(\alpha - k_1)^2 + q_2^2 > 0$$

Substituting

$$y = r\cos\theta\ ,\ z_2 = r\sin\theta$$

we get

$$\frac{1}{2}\, H(\alpha) = \int_0^\infty \frac{re^{iq(r^2+z_3^2)^{1/2}}}{(r^2 + z_3^2)^{1/2}} \left[\int_0^{\pi/2} \cos((\alpha - q_1)r\cos\theta) \cos(q_2 r \sin\theta) d\theta \right]\, dr.$$

We can write

$$\begin{aligned} &2\cos((\alpha - q_1)r\cos\theta)\cos(q_2 r\sin\theta) \\ &= \cos((\alpha - q_1)r\cos\theta + q_2 r\sin\theta) + \cos((\alpha - q_1)r\cos\theta - q_2 r\sin\theta) \\ &= \cos(Ar\cos(\theta + \phi_1)) + \cos(Ar\cos(\theta + \phi_2)), \quad A = \sqrt{(\alpha - q_1)^2 + q_2^2} \end{aligned}$$

for suitable angles ϕ_1, ϕ_2. Noting that

$$\int_0^{\pi/2} \cos((\alpha - q_1)r\cos\theta)\cos(k_2 r\sin\theta)d\theta$$

is equal to each of the integrals

$$\int_{\pi/2}^{\pi},\quad \int_{\pi}^{3\pi/2},\quad \int_{3\pi/2}^{2\pi}$$

with the same integrand, we get

$$\begin{aligned} &\int_0^{\pi/2} \cos((\alpha - q_1)r\cos\theta)\cos(q_2 r\sin\theta)d\theta \\ &= \frac{1}{8}\{\int_0^{2\pi} \cos(Ar\cos(\theta + \phi_1))d\theta + \int_0^{2\pi} \cos(Ar\cos(\theta + \phi_2))d\theta\} \\ &= \frac{1}{4}\int_0^{2\pi} \cos(Ar\cos\theta)d\theta = \int_0^{\pi/2} \cos(Ar\cos\theta)d\theta. \\ &= \frac{\pi}{2} J_0(Ar), \end{aligned}$$

by formula #19 in p. 402 of [8]. We deduce that

$$\frac{1}{2}H(\alpha) = \frac{\pi}{2}\int_0^\infty \frac{re^{iq(r^2+z_3^2)^{1/2}}}{(r^2+z_3^2)^{1/2}}\, J_0(Ar)\, dr, \quad A = \sqrt{(\alpha-q_1)^2+q_2^2}.$$

We can evaluate the right–hand side by formula (21) of [6; p. 31] with $\nu = 0$, $a = k, x = r, y = A$; setting

$$\tilde{\alpha} = \sqrt{(\alpha-q_1)^2+q_2^2}$$

we conclude that

$$\frac{1}{2}\, H(\alpha) = i\frac{\pi 2^{-1/2}\pi^{1/2}}{2\tilde{\alpha}^{1/2}}\, |z_3|^{1/2}(q^2-\tilde{\alpha}^2)^{-1/4}\tilde{\alpha}^{1/2}H^{(1)}_{-\frac{1}{2}}[|z_3|(q^2-\tilde{\alpha}^2)^{1/2}] \quad \text{if} \quad 0<|\tilde{\alpha}|<q\,, \tag{2.13}$$

$$\frac{1}{2}\, H(\alpha) = \frac{\pi 2^{1/2}\pi^{-1/2}}{2\tilde{\alpha}^{1/2}}\, |z_3|^{1/2}\tilde{\alpha}^{1/2}(\tilde{\alpha}^2-q^2)^{-1/4}K_{\frac{1}{2}}[|z_3|(\tilde{\alpha}^2-q^2)^{1/2}] \quad \text{if} \quad q<|\tilde{\alpha}|<\infty\,. \tag{2.14}$$

By [9; p. 73],

$$\begin{aligned} H^{(1)}_{-\frac{1}{2}}(z) &= \left(\frac{1}{2}\,\pi z\right)^{-1/2} e^{iz}\,, \\ K_{\frac{1}{2}}(z) &= \left(\frac{\pi}{2z}\right)^{1/2} e^{-z}\,. \end{aligned} \tag{2.15}$$

Hence

$$H(\alpha) = \frac{\pi i}{(q^2-\tilde{\alpha}^2)^{1/2}}e^{i(q^2-\tilde{\alpha}^2)^{1/2}|z_3|} \qquad \text{if} \qquad 0<|\tilde{\alpha}|<q, \tag{2.16}$$

$$H(\alpha) = \frac{\pi}{(\tilde{\alpha}^2-q^2)^{1/2}}e^{-(\tilde{\alpha}^2-q^2)^{1/2}|z_3|} \qquad \text{if} \qquad q<|\tilde{\alpha}|<\infty. \tag{2.17}$$

Consider next the case when $(\alpha-q_1)^2+q_2^2 = 0$, i.e., $\tilde{\alpha} = 0$. Then

$$\begin{aligned} H(\alpha) &= \int_0^\infty F(q_1, z_2, z_3)\, dz_2 \\ &= 2\int_0^\infty\int_0^\infty \frac{e^{iq(y^2+z_2^2+z_3^2)^{1/2}}}{(y^2+z_2^2+z_3^2)^{1/2}}\, dy\, dz_2\,. \\ &\equiv 2\int_0^\infty D(y, z_3)\, dy\,. \end{aligned}$$

Setting $t^2 = y^2 + z_3^2$ and substituting $\zeta = (t^2 + z_2^2)^{\frac{1}{2}}/t$, we get

$$D(y, z_3) = \int_1^\infty \frac{e^{iqt\zeta}}{\sqrt{\zeta^2 - 1}}\, d\zeta \ .$$

Using formulas §3.743 #3 and #4 of [8; p. 419], we find that

$$D(y, z_3) = -\frac{\pi}{2}\, N_0(qt) + \frac{\pi i}{2}\, J_0(qt)$$

where N_0 is the Neumann function. From [8; p. 951] formula §8.405 #1 we then get

$$D(y, z_3) = \frac{\pi i}{2}\, H_0^{(1)}(qt)$$

where $H_0^{(1)}$ is a Hankel function. Substituting this into (3.3), we get

$$H(\alpha) = \pi i \int_0^\infty H_0^{(1)}[q(y^2 + z_3^2)^{1/2}]\, dy\ , \qquad \tilde{\alpha} = 0$$

Substituting $y = t|z_3|$ and then $t^2 + 1 = s$, we find that

$$\begin{aligned} H(\alpha) &= \frac{\pi i}{2}\, |z_3| \int_1^\infty H_0^{(1)}(q|z_3|\sqrt{s}) \frac{ds}{\sqrt{s-1}} \\ &= \frac{\pi i}{2}\, |z_3|\sqrt{2}(q|z_3|)^{-1/2} H_{-\frac{1}{2}}^{(1)}(q|z_3|)\Gamma(\frac{1}{2}\ ) \end{aligned}$$

where the last relation is due to [8; p. 703 # 14]. Using the formula in [10; p. 73] for $H_{-1/2}^{(1)}$ we finally get the estimate

$$H(\alpha) = \frac{\pi i}{q}\, e^{iq|z_3|} \qquad \text{if} \qquad \tilde{\alpha} = 0 \quad (\text{i.e., } \alpha = q_1 \text{ and } q_2 = 0). \tag{2.19}$$

Thus, (2.15) is valid also when $\tilde{\alpha} = 0$.

Clearly $B_m = 0$ if m is even; if m is odd then, as easily verified,

$$\int_{x_1}^{x_1 + L/2} B_m(t)\, dt = \frac{4i}{\pi m}\, e^{-i\frac{2\pi m}{L}\, x_1}\ .$$

We shall assume from now on that

$$(q_1 - \frac{2\pi m}{L})^2 + q_2^2 \neq q^2 \quad \text{for all integers } m,$$

i.e.,

$$(q_1 - \frac{2\pi m}{L})^2 \neq q_1^2 + q_3^2.$$

This means that there exists a positive constant σ such that

$$|(q_1 - \frac{2\pi m}{L})^2 + q_2^2 - q^2| \geq \sigma > 0 \quad \forall m = 0, 1, 2, \ldots \tag{2.20}$$

We conclude that there exists an integer $m_0 \geq 0, m_1 \geq 0$ such that

$$\begin{aligned} &(q_1 - \frac{2\pi m}{L})^2 + q_2^2 < q^2 \quad \text{if} \quad -m_1 \leq m \leq m_0, \\ &(q_1 - \frac{2\pi m}{L})^2 + q_2^2 > q^2 \quad \text{if} \quad -\infty < m \leq -m_1 - 1 \quad \text{or if} \quad m_0 + 1 \leq m < \infty. \end{aligned} \tag{2.21}$$

Set

$$\alpha_m = \left\{ q^2 - \left(\frac{2\pi m}{L} - q_1 \right)^2 - q_2^2 \right\}^{1/2}. \tag{2.22}$$

Substituting (2.16), (2.17) (2.19) into (2.11) and using the resulting expression in (2.4), we get

$$J_*(X) = -2 \sum_{\substack{m=-\infty \\ m \text{ odd}}}^{\infty} \frac{4}{m\alpha_m} e^{-i\frac{2m\pi x_1}{L}} e^{i\alpha_m |z_3|}. \tag{2.23}$$

Since J_* is the inner integral in the right–hand side of (2.2), we get

$$\begin{aligned} (K1)(X) = m = \frac{2}{\pi} \sum_{\substack{m=-\infty \\ m \text{ odd}}}^{\infty} \frac{1}{m\alpha_m} e^{-i\frac{2\pi m x_1}{L}} \\ \cdot \int_{x_3-d/2}^{x_3+d/2} e^{-iq_3 z_3} e^{i\alpha_m |z_3|} \quad dz_3. \end{aligned} \tag{2.24}$$

As easily verified, if $-\frac{d}{2} < x_3 < \frac{d}{2}$ then

$$\begin{aligned} \int_{x_3-d/2}^{x_3+d/2} e^{-iq_3 z_3} e^{i\alpha_m |z_3|} \, dz_3 = -\frac{2i\alpha_m}{q^2 - \alpha_m^2} \\ + e^{-i(q_3+\alpha_m)x_3} \frac{e^{i(q+\alpha_m)d/2}}{iq_3 + i\alpha_m} + e^{i(\alpha_m - q_3)x_3} \frac{e^{i(\alpha_m - q)\, d/2}}{-iq_3 + i\alpha_m}. \end{aligned} \tag{2.25}$$

Substituting this into (2.24) we get

$$(2.26)\quad \begin{aligned}(K1)(X) = \frac{2}{\pi} \sum_{\substack{m=-\infty \\ m \text{ odd}}}^{\infty} \frac{1}{m\alpha_m} e^{-i\frac{2\pi m x_1}{L}} \Bigg[&-\frac{2i\alpha_m}{q_3^2 - \alpha_m^2} \\ &+ e^{-i(\alpha_m+q_3)x_3} \frac{e^{i(q_3+\alpha_m)d/2}}{iq_3 + i\alpha_m} + e^{i(\alpha_m-q_3)x_3} \frac{e^{i(\alpha_m-q_3)d/2}}{-iq_3 + i\alpha_m} \Bigg]\end{aligned}$$

for $-\frac{d}{2} < x_3 < \frac{d}{2}$ provided $q_3^2 \neq \alpha_m^2$ for all m odd, i.e., provided

$$(2.27)\qquad q_1 \neq \frac{m\pi}{L} \quad \forall m \quad \text{odd}.$$

If $q_1 = \frac{m\pi}{L}$ for some $m = \tilde{m}$, $\tilde{m}$ odd, then (2.25) takes a different form for $m = \tilde{m}$ and there is a corresponding change for the terms with $m = \tilde{m}$ in (2.20). This however does not affect the subsequent analysis and therefore, for simplicity, we assume in the sequel that (2.27) holds, so that (2.26) is valid.

Next, we easily obtain from (2.24),

$$(2.28)\quad (K1)(X) = \frac{d/2}{\pi} \sum_{\substack{-m_1 \leq m \leq m_0 \\ m \text{ odd}}} \frac{\sin((q_3 - \alpha_m)d/2)}{m\alpha_m(q_3 - \alpha_m)} e^{-i\frac{2\pi m x_1}{L}} e^{i(\alpha_m - q_3)x_3} + O(e^{-\gamma|x_3|}) \quad \text{if} \quad x_3 > \frac{d}{2}$$

and

$$(2.29)\quad (K1)(X) = \frac{d/2}{\pi} \sum_{\substack{-m_1 \leq m \leq m_0 \\ m \text{ odd}}} \frac{\sin((q_3 + \alpha_m)d/2)}{m\alpha_m(q_3 + \alpha_m)} e^{-i\frac{2\pi m x_1}{L}} e^{-i(\alpha_m + q_3)x_3} + O(e^{-\gamma|x_3|}) \quad \text{if} \quad x_3 < -\frac{d}{2}$$

where γ is some positive constant.

§3. Evaluation of Kf. Consider the expression

$$(3.1)\qquad I(s_1 z_3) \equiv \int_0^\infty \sum_{n=-\infty}^{\infty} e^{-iq_1(s+nL)} e^{-iq_2 z_2} \frac{e^{ik[(s+nL)^2 + z_2^2 + z_3^2]^{1/2}}}{[(s+nL)^2 + z_2^2 + z_3^2]^{1/2}} \, dz_2$$

which is precisely

$$\sum_{n=-\infty}^{\infty} G(s+nL,\ z_3), \qquad G \quad \text{as in (2.3)}.$$

Using the Poisson summation formula as before, we find that

$$I(s,z_3) = \frac{1}{L}\int_0^{\infty} \sum_{m=-\infty}^{\infty} F\left(\frac{2\pi m}{L}, z_2, z_3\right) e^{-i\frac{2\pi m s}{L}}\, dz_2$$

and, by (2.12), (2.16), (2.17) and (2.19),

$$I(s,z_3) = \sum_{m=-\infty}^{\infty} \frac{1}{L} e^{-i\frac{2m\pi s}{L}} \frac{\pi i}{\alpha_m} e^{i\alpha_m |z_3|}\ . \tag{3.2}$$

We can now compute Kf when $f(x_1,x_3)$ is any bounded function, periodic in x_1 of period L. Since $V(x_1)$ is also L–periodic, we easily find that

$$\begin{aligned} Kf &= -\frac{1}{4\pi}\int_{-d/2}^{d/2} d\eta \int_{x_1-L}^{x_1} e^{-iq_3(x_3-\eta)} I(x_1-\tau, x_3-\eta)\widetilde{V}(\tau) f(\tau,\eta)\, d\eta \\ &= -\frac{1}{4\pi L}\int_{-d/2}^{d/2} d\eta \int_{x_1-L}^{x_1} \sum_{m=-\infty}^{\infty} e^{-i\frac{2\pi m(x_1-\tau)}{L}} \\ &\qquad \cdot \frac{\pi i}{\alpha_m} e^{-iq_3(x_3-\eta)} e^{i\alpha_m|x_3-\eta|}\widetilde{V}(\tau) f(\tau,\eta)\, d\tau\ , \end{aligned}$$

by (3.2). Further

$$\int_{x_1-L}^{x_1} e^{i\frac{2\pi m\tau}{L}} \widetilde{V}(\tau) f(\tau,\eta)\, d\tau = \gamma_m(\eta) \tag{3.3}$$

where $\gamma_m(\eta)$ is independent of x_1 since the integrand is L–periodic in τ. Hence

$$Kf = -\frac{i}{4L}\sum_{m=-\infty}^{\infty} \frac{1}{\alpha_m} e^{-i\frac{2\pi m x_1}{L}} \int_{-d/2}^{d/2} e^{-iq_3(x_3-\eta)} e^{i\alpha_m|x_3-\eta|} \gamma_m(\eta)\, d\eta \tag{3.4}$$

and $|\gamma_m(\eta)| \le C$; the change of order of integration is justified since the series is convergent in the norm of the space B defined in §1. If $x_3 > d/2$ then we get

$$(Kf)(x_1,x_3) = -\frac{i}{4L}\sum_{m=-\infty}^{\infty} \frac{\beta_m}{\alpha_m} e^{-i\frac{2\pi m x_1}{L}} e^{i(\alpha_m - q_3)x_3} \tag{3.5}$$

where

$$\beta_m = \int_{-d/2}^{d/2} e^{-i(\alpha_m+q_3)\eta}\gamma_m(\eta)\, d\eta \; ; \tag{3.6}$$

clearly

$$\left|\frac{\beta_m}{\alpha_m}\right| \le \frac{C}{|m|+1} \, . \tag{3.7}$$

Noting that

$$|e^{i\alpha_m x_3}| \le C\; e^{-\gamma|m|x_3} \quad \text{if} \quad m \notin [-m_1, m_0], x_3 > 0 \tag{3.8}$$

for some $\gamma > 0$, it follows that

$$\begin{aligned}(Kf)(x_1,x_3) = -\frac{i}{4L} \sum_{m=-m_1}^{m_0} \frac{\beta_m}{\alpha_m}\, e^{-i\frac{2\pi m x_1}{L}}\, e^{i(\alpha_m - q_3)x_3} \\ + O(e^{-\gamma x_3}) \quad \text{if} \quad x_3 > \frac{d}{2} \, .\end{aligned} \tag{3.9}$$

A similar asymptotic formula holds for $x_3 < -\frac{d}{2}$.

§4. Compactness of K; solution of (1.6).

THEOREM 4.1. *The operator K is a compact bounded linear operator in the space B.*

Proof. From (3.5), (3.3), (3.6) we see that K maps B into itself. Let

$$K_n f = -\frac{i}{4L} \sum_{m=-n}^{n} \frac{1}{\alpha_m}\, e^{-i\frac{2\pi m x_1}{L}} \int_{-d/2}^{d/2} e^{-iq_3(x_3-\eta)} e^{i\alpha_m|x_3-\eta|}\gamma_m(\eta)\, d\eta \, .$$

Since K_n has a finite dimensional range, it is clearly a compact bounded linear operator; to prove that K is a compact bounded linear operator it suffices to show that

$$K_n \to K \quad \text{in the uniform norm.} \tag{4.1}$$

But

$$(K_n - K)f = -\frac{i}{4L} \sum_{|m|>n} \frac{1}{\alpha_m}\, e^{-i\frac{2\pi m x_1}{L}} \int_{-d/2}^{d/2} e^{iq_3(x_3-\eta)} e^{i\alpha_m|x_3-\eta|}\gamma_m(\eta)\, d\eta$$

and, by Bessel's inequality, we easily get

$$\|(K_n - K)f\|_{L^2(0\le x_1\le L)} \le C\|f\| \sum_{|m|>n} \frac{1}{|\alpha_m|^2} \, .$$

Thus

$$\|K_n - K\| \le C \sum_{|m|>n} \frac{1}{|\alpha_m|^2} \to 0 \quad \text{if} \quad n \to \infty,$$

and (4.1) follows.

As mentioned in §1, the Fredholm alternative can now be applied to K. If we denote by W_j the (at most) countable set of positive eigenvalues of K $\quad (W_j \to \infty$ if $j \to \infty)$ then we have:

THEOREM 4.2. *If $V_0 \neq W_j \quad \forall j$ then for any $f \in B$ there exists a unique solution ϕ of (1.14) in B.*

From the formulas derived for $K\phi \quad (\phi \in B)$ in §3 it follows that

$$e^{i\vec{q}\cdot X}(\phi - f)$$

has the expansion (1.9) without the first term $e^{i\vec{q}\cdot X}$ and with

$$|T_n| \le \frac{C}{|n|+1} \quad , \; |R_n| \le \frac{C}{|n|+1} \, ; \tag{4.2}$$

in view of (3.8), the series in (1.9) are absolutely uniformly convergent in $\{x_3 \ge \frac{d}{2} + \epsilon\}$, $\{x_3 \le -\frac{d}{2} - \epsilon\}$, for any $\epsilon > 0$.

Taking, in particular, $f = 1$ we conclude that, if $V_0 \neq W_j$ for all j, then equation (1.5) has a unique solution and the expansion (1.9) holds with T_n, R_n satisfying (4.2). The proof of the expansion, however, is not constructive and does not provide a means for computing T_n, R_n.

§5. The case of $\mathbf{V_0}$ small.

In this section we shall compute the transmission and reflection coefficients in case V_0 is sufficiently small, i.e.,

$$V_0 d \le \frac{1}{C} \tag{5.1}$$

where C is some positive constant depending only on $\vec{q}$. The method is based on the Neumann series

$$(I - V_0 K)^{-1} = I + \sum_{n=1}^{\infty} V_0^n K^n$$

or, equivalently, on successive iterations in the integral equation (1.5) or, rather, (1.16).

We begin with:

THEOREM 5.1. *There exists a positive constant depending only on σ, m_0, m_1 (defined in (2.20), (2.21)) such that if (5.1) holds then there exists a unique bounded solution Φ of equation (1.5) having the form (1.12).*

REMARK 5.1. The novelty of the theorem is that it provides an estimate on the smallest eigenvalue W_1, i.e., $W_1 > (Cd)^{-1}$. This can also be derived rather quickly from the expression for Kf in §3. However, the proof of Theorem 5.1 will be needed later on.

Proof. We shall construct a solution of (1.16) of the form

$$\phi(x_1, x_2) = 1 + \sum_{n=1}^{\infty} \phi_n\ (x_1, x_3) \tag{5.2}$$

where ϕ_j are defined iteratively by

$$\phi_{n+1}(X) = -\frac{1}{4\pi} \int\limits_{\mathbf{R}^3} e^{-i\vec{q}\cdot(X-Y)} \frac{e^{iq|X-Y|}}{|X-Y|} V(Y)\phi_n(Y)dY\ . \tag{5.3}$$

Clearly ϕ is formally a solution of (1.16). To prove this rigorously we shall establish the estimates

$$|\phi_n(X)| \le C^n V_0^n d^n \tag{5.4}$$

where C is a positive constant dependent only on m_0, m_1, σ. The proof for $n = 1$ follows from the form for $K1$ derived in §2.

It is easily verified that if ϕ_n is a function of (x_1, x_3) only, periodic in x_1 of period L, then the same is true of ϕ_{n+1} , and

$$\phi_{n+1}(x_1, x_3) = -\frac{1}{4\pi} \int\limits_{x_3-d/2}^{x_3+d/2} dz_3 \int\limits_{x_1-L}^{x_1} d\tau \int\limits_{-\infty}^{\infty} \sum_{m=-\infty}^{\infty}$$

$$e^{iq_1(x_1-\tau+mL)} e^{-i(q_2 z_2 + q_3 z_3)} \frac{e^{iq[(x_1-\tau+mL)^2+z_2^2+z_3^2]^{1/2}}}{[(x_1-\tau+mL)^2+z_2^2+z_3^2]^{1/2}} V(\tau)\phi_n(\tau, x_3 - z_3)\ dz_2.$$

Using (3.2) we get

$$(5.5)\qquad \phi_{n+1}(x_1,x_3) = -\frac{i}{2L}\int\limits_{x_3-d/2}^{x_3+d/2} dz_3 \int\limits_{x_1-L}^{x_1} \left[\sum_{m=-\infty}^{\infty} \frac{1}{\alpha_m} e^{i\,\alpha_m|z_3|}\right] V(\tau)\phi_n(\tau, x_3 - z_3)\,d\tau.$$

In view of (2.21), (2.22)

$$(5.6)\qquad \Big|\sum_{\substack{m=-\infty\\ m\notin[-m_1,m_0]}}^{\infty} \frac{1}{\alpha_m} e^{-i\frac{2\pi m(x_1-\tau)}{L}} e^{i\alpha_m|z_3|}\Big| \le Ce^{-\gamma|x_3|},$$

where C, γ are positive constants. Using (5.4) in (5.5) and using also (5.6), we easily obtain the inequality (4.3) for $n+1$.

To prove uniqueness suppose Φ_* is another bounded solution of the form (1.12), (5.2), (5.3), say $\Phi_* = e^{i\vec{q}\cdot X}\phi_*$, and set $\psi = \phi - \phi_*$. Then

$$\psi(x_1,x_2) = -\frac{1}{4\pi}\int\limits_{\mathbf{R}^3} e^{-i\vec{q}\cdot(X-Y)}\frac{e^{iq|X-Y|}}{|X-Y|} V(Y)\psi(y_1,y_2)\,dY.$$

Arguing as in the proof of (5.4) we deduce that

$$\sup|\psi| \le CV_0 d\cdot \sup|\psi|\ ,$$

so that $\psi \equiv 0$.

THEOREM 5.2. *If (5.1) holds for a suitable constant C depending only on m_0, m_1, σ, then the solution of (1.5) has the form (1.9) with*

$$(5.7)\qquad |T_n| \le \frac{C_0}{|n|+1}\ ,\ |R_n| \le \frac{C_0}{|n|+1}$$

where C_0 is a constant.

Remark 5.2. If $x_3 > d/2$ then

$$|e^{e^{i\vec{q}_n^+\cdot X}}| \le C_1 e^{-\gamma|n|x_3} \qquad \text{if} \qquad |n| \le m_1 - 1 \quad \text{or if } n \ge m_0+1$$

where C_1, γ are positive constants. Hence from (1.9) and (5.7) it follows that

$$(5.8)\qquad \Phi(X) = e^{i\vec{q}\cdot X} + \sum_{\substack{n=-\infty\\ n\notin[-m_1,m_0]}}^{\infty} T_n e^{i\vec{q}_n^+\cdot X} + O(e^{-\gamma x_3}) \quad \text{if} \quad x_3 > \frac{d}{2}.$$

Similarly

$$(5.9)\qquad \Phi(X) = \sum_{\substack{n=-\infty \\ n\notin[-m_1,m_0]}}^{\infty} R_n e^{i\vec{q}_n^{\,-}\cdot X} + O(e^{-\gamma|x_3|}) \quad \text{if} \quad x_3 < -\frac{d}{2}.$$

Proof. We shall need the formula

$$(5.10)\qquad \int_{x_1-L}^{x_1} e^{i\frac{2\pi j\tau}{L}} V(\tau)d\tau = \begin{cases} 0 & \text{if } j \text{ is even} \\ \dfrac{2iV_0}{\pi j} & \text{if } j \text{ is odd.} \end{cases}$$

We shall prove by induction on n that

$$(5.11)\qquad \phi_n(x_1, x_3) = \sum_{m=-\infty}^{\infty} \Gamma_m^n(x_3) e^{i\frac{2\pi m x_1}{L}},$$

$$(5.12)\qquad |\Gamma_m^n(x_3)| \le \frac{C^n V_0^n d^n}{|m|+1}$$

where C is a suitable constant. Indeed, by (2.26), this is true for $n = 1$. Assuming that (5.11), (5.12) hold for some $n \ge 1$ we proceed to derive the same expansion for ϕ_{n+1} by using (5.5).

Substituting ϕ_n from (5.11) into (5.5) and using (5.10), we easily obtain the expansion (5.11) for ϕ_{n+1} with

$$|\Gamma_m^{n+1}| \le \sum_{j=-\infty}^{\infty} \frac{C_2}{|m-j|+1} \frac{1}{|\alpha_m|} \frac{C^n V_0^n d^n}{|j|+1} V_0 d \quad ;$$

C_j will be used to denote various constants; the last factor d comes from the integration with respect to z_3. Since $|\alpha_m| \ge c(|m|+1), c > 0$,

$$\sum_{j=-\infty}^{\infty} \frac{1}{(|m-j|+1)|\alpha_m|(|j|+1)} \le \frac{C_3}{|m|+1},$$

and the estimate (5.12) follows for Γ_m^{n+1}.

We now proceed to evaluate the $\phi_n(x_1, x_3)$ for $x_3 > \frac{d}{2}$. Substituting $x_3 - z_3 = \eta$ in the right–hand side of (5.5), we get

(5.6)

$$\phi_{n+1}(x_1, x_3) = -\frac{i}{2L} \int_{-d/2}^{d/2} d\eta \Big\{ \int_{x_1-L}^{x_1} \sum_{m=-\infty}^{\infty} \frac{1}{\alpha_m} e^{-i\frac{2\pi m(x_1-\tau)}{L}} e^{-iq_3(x_3-\eta)} e^{i\alpha_m(x_3-\eta)} \Big\} V(\tau)\phi_n(\tau, \eta)\, d\tau$$

since $|x_3 - \eta| = x_3 - \eta$. Noting that

$$|e^{i\alpha_m(x_3-\eta)}| \leq C_4 e^{-\gamma m} \qquad \text{if} \quad m > m_0 \quad \text{or } m < -m_1$$

where γ is a positive constant, we see that the series in (5.13) is absolutely uniformly convergent. Hence we can change the order of integration as well as integrate term–by–term. Consequently, we can write

$$\begin{aligned} &\phi_{n+1}(x_1, x_3) = \\ (5.14) \qquad &-\frac{i}{2L}\sum_{m=-\infty}^{\infty} \frac{e^{i(\alpha_m - q_3)x_3}}{\alpha_m} \int_{x_1-L}^{x_1} e^{-i\frac{2\pi m(x_1-\tau)}{L}} V(\tau)\psi_n(\tau)d\tau \end{aligned}$$

where

$$\begin{aligned} \psi_n(\tau) &= \int_{-d/2}^{d/2} e^{i\alpha_m \eta} e^{iq_3\eta}\phi_n(\tau,\eta)d\eta \\ (5.15) \qquad &= \sum_{j=-\infty}^{\infty} \tilde{\Gamma}_j^n e^{i\frac{2\pi j\tau}{L}}, \quad \text{by (5.11)} \end{aligned}$$

and

$$|\tilde{\Gamma}_j^n| \leq C_5 \frac{C^n V_0^n d^{n+1}}{|j|+1}, \quad \text{by (5.12).}$$

Substituting (5.15) into (5.14) and using (5.10), we get

$$(5.16) \qquad \phi_{n+1}(x_1, x_3) = \sum_{m=-\infty}^{\infty} \gamma_m^n e^{i(\alpha_m - q_3)x_3} e^{-i\frac{2m\pi}{L}x_1}$$

where

$$|\gamma_m^n| \leq C_0 \frac{C^n V_0^{n+1} d^{n+1}}{m+1}.$$

Assuming that C is such that $CV_0 d < 1$ and summing on n (in (5.2)), the assertion (1.9) follows for $x_3 > \frac{d}{2}$, with T_n satisfying (5.7). The proof for $x_3 < -\frac{d}{2}$ is similar.

Remark 5.3. The coefficients T_m, R_m can be computed as follows. First we compute the ϕ_n inductively from (5.5). Next we compute the Γ_m^n in (5.11) as the Fourier coefficients of ϕ_n. Finally we compute the ψ_n by (5.15) and the γ_m^n as explained above, using (5.10). Once the γ_m^n have been computed, summation on n yields the coefficients T_m. The R_m are computed similarly.

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