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Scattering of Waves by Irregularities in Periodic Discrete Lattice Spaces. I. Reduction of Problem to Quadratures on a Discrete Model of the Schrödinger Equation

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The scattering of plane waves and of point source pulses by irregularities in a discrete lattice model of the Schrödinger equation is considered. Closed form expressions are derived for the scattered wave function in terms of lattice Green's functions in the case that a finite number of lattice points or "bonds" are defective. The scattered wave function appears in the form of the ratio of two determinants. While in continuum scattering theory the scatterer must have some symmetry, perhaps spherical, cylindrical or elliptical, in order to allow separation of variables in the basic scattering differential equation, such symmetries are not necessary for the construction of scattered wave functions on discrete lattices. When the number of irregularities becomes large, the determinants in the solution of the scattering problem become large.

KEY WORDS: Scattering theory; defects; lattice statistics.

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1. INTRODUCTION

Waves propagating in a medium are scattered by irregularities in that medium. Thus waves of sound, light, neutrons, and electrons are scattered by density fluctuations in condensed phases of matter; electromagnetic waves are scattered by electron density fluctuations in the ionosphere; protons and electrons are scattered by atomic nuclei, etc. The pattern of the scattered wave provides one of the most important bits of information for the deduction of the nature of the irregularity. Unfortunately, in few cases has the scattering theory been developed and presented sufficiently clearly and precisely so that an accurate analysis of the scattering process can be easily made. Even in one of those few cases in which a scattering problem is solved "exactly," the Mie theory of scattering of an electromagnetic wave by a uniform sphere, the final analysis of the exact formulas may become a tremendous tour de force, as is witnessed in the outstanding papers of Nussenzveig.[1]

Through some experience in investigating the wave propagation in discrete media such as crystal lattices[2–4] it has been noticed that while free "particle" propagators are more complicated on lattices, the scattering formulas become simpler and easier to interpret. The reason for this is that on a lattice the approach to and retreat from the surface of a defect region can be made in only a limited number of directions. Internal reflections in the defect regions are easier to characterize. In the case of a finite number of defect points in a discrete medium the full scattering problem can be reduced to the solution of a number of linear algebraic equations which is of the order of the number of defect points.

The aim of this paper is to derive relatively simple closed form expressions, usually in the form of determinants, for scattered wave functions in irregular discrete media. These formulas will later be used in other reports to generate, in a concise way, scattering patterns resulting from a wide variety of irregularities. While most real scatterers of interest are continuous, it will be found that many qualitative features of scattering processes can be deduced more easily from discrete models. All formulas will be expressed in terms of lattice Green's functions, quantities which have been the subject of a number of recent investigations.[10–15]

This paper is an exposition of the general method of deriving the basic formulas which will be used later for detailed analyses. It will not be developed in terms of any specific physical problem of interest but rather in terms of a simple prototype model which will be chosen to be the discrete analog of the Schrödinger equation so that the scattering theory will be the analog of quantum mechanical scattering by a potential. However, we shall also consider the case of several disconnected scattering regions so that formulas for interference patterns of several separated scattering centers can be discussed.

While the standard theories of scattering emphasize the scattering of plane waves, we will begin our presentation with the scattering of a point source instantaneous pulse by an irregularity since the mathematics of this problem is almost identical with that already used to study the effect of defects on the random walk of a walker on a lattice.[5,6] We will then proceed with a discussion of scattering of plane waves by lattice defects.

2. A DISCRETE MODEL SIMILAR TO NONRELATIVISTIC QUANTUM THEORY

We devote this section to the characterization of our empty discrete lattice space. Consider first a classical random walk on a one-dimensional continuum without defects. Let $P(x, t)$ be the probability distribution function for the location of a walker. This function is nonnegative and normalized to unity. The transition probability $p(x, \tau)$ for a displacement from x_0 to x in a time τ gives the relation between $P(x, t + \tau)$ and $P(x_0, t)$:

$$P(x, t + \tau) = \int_{-\infty}^{\infty} p(x - x_0; \tau)P(x_0, t)\, dx_0 \tag{1}$$

Let us suppose that at some intermediate time $\tau < \tau'' < t$ the walker goes through some point x_1; then

$$P(x_1, \tau'') = \int_{-\infty}^{\infty} p(x_1 - x_0; \tau'' - t)P(x_0, t)\, dx_0$$

and

$$\begin{aligned} P(x, t + \tau) &= \int_{\infty}^{\infty} p(x - x_1, t + \tau - \tau'')P(x_1, \tau'')\, dx_1 \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p(x - x_1, t + \tau - \tau'') \\ &\qquad \times p(x_1 - x_0, \tau'' - t)P(x_0, t)\, dx_1\, dx_0 \end{aligned} \tag{2}$$

Hence if we compare (1) and (2), with $\tau' \equiv (\tau'' - t)$, we obtain the well-known Chapman–Kolmogoroff–Smoluchowski chain condition, which was actually first discussed by Bachelier in 1900 in his Ph.D. thesis (on the stock market and directed by Poincaré).

$$p(x - x_0; \tau) = \int_{-\infty}^{\infty} p(x - x_1, \tau - \tau')p(x_1 - x_0, \tau')\, dx_1 \tag{3}$$

The quantum mechanical analog of (1) is the equation that relates a wave function $\psi(x, t + \tau)$ to $\psi(x_0, t)$ through the propagator $K(x, t)$:

$$\psi(x, t + \tau) = \int_{-\infty}^{\infty} K(x - x_0; \tau)\psi(x_0, t)\, dx_0 \tag{4}$$

It is easy to see that the propagator[7] also satisfies the chain condition

$$K(x - x_0; \tau) = \int_{-\infty}^{\infty} K(x - x_1, \tau - \tau')K(x_1 - x_0; \tau')\, dx_1 \tag{5}$$

as well as the unitarity condition

$$\int_{-\infty}^{\infty} K(x - x_0; t)K^*(x - x_1; t)\, dx = \delta(x_1 - x_0) \tag{6}$$

which is necessary to preserve probability normalization in quantum theory

$$\int_{-\infty}^{\infty} |\psi(x, t + \tau)|^2\, dx = \int_{-\infty}^{\infty} |\psi(x_0, t)|^2\, dx_0 = 1 \tag{7}$$

The classical Gaussian transition probability

$$p(x, t) = \begin{cases} (4\pi Dt)^{-1/2} \exp(-x^2/4Dt), & t \geqslant 0 \\ 0, & t < 0 \end{cases} \tag{8}$$

satisfies (3) and the quantum mechanical free particle propagator

$$K(x, t) = \begin{cases} (4\pi\lambda it)^{-1/2} \exp(-ix^2/4\lambda t), & t \geqslant 0 \\ 0, & t < 0 \end{cases} \tag{9}$$

satisfies the chain condition (5) as well as the unitarity condition (6). The Gauss distribution (8) is the Green's function of the diffusion equation

$$P_t - DP_{xx} = \delta(x)\, \delta(t) \tag{10}$$

and the propagator (9) is the Green's function of the free particle Schrödinger equation

$$K_t + i\lambda K_{xx} = \delta(x)\, \delta(t) \qquad \text{with} \quad \lambda = \hbar/2m \tag{11}$$

Now consider a one-dimensional discrete system of N points on a ring (periodic boundary conditions). Let the successive points on the ring be denoted by 0, 1, 2,..., N − 1 (with $N \equiv 0$). Then the analog of the chain condition (3) becomes

$$p(l - l_0, \tau) = \sum_{l_1=1}^{N} p(l - l_1, \tau - \tau')p(l_1 - l_0, \tau') \tag{12}$$

with a similar analog existing to (5). The transition probability function

$$p_0(l, t) = \frac{1}{N} \sum_{s=1}^{N} \exp\left[\frac{2\pi i l s}{N} - 2\alpha t \left(1 - \cos\frac{2\pi s}{N}\right)\right] \qquad \text{if} \quad t > 0 \tag{13}$$

can be shown to satisfy (12) by analyzing the right-hand side of (12):

$$\frac{1}{N^2} \sum_{l_1=1}^{N} \sum_{s_1=1}^{N} \sum_{s_2=1}^{N} \exp\left\{\frac{2\pi i[(l - l_1)s_1 + (l_1 - l_0)s_2]}{N}\right\}$$
$$\times \exp\left\{2\alpha\left[(\tau - \tau') \cos\left(\frac{2\pi s_1}{N}\right) + \tau' \cos\left(\frac{2\pi s_2}{N}\right) - \tau\right]\right\} \tag{14}$$

Since

$$(1/N)\sum_{l_1=1}^{N}\exp[2\pi i l_1(s_2 - s_1)/N] = \delta_{s_1 s_2} \tag{15}$$

we find that (14) becomes

$$(1/N)\sum_{s=1}^{N}\exp[2\pi i(l - l_0)s/N]\exp\{-2\alpha\tau[1 - \cos(2\pi s/N)]\}$$

which is exactly (13) with t replaced by τ as required.

The slightly more general transition probability

$$p_0(l, t) = H(t)N^{-1}\sum_{s=1}^{N}\exp\left[\frac{2\pi i l s}{N} - 2\alpha t\left(1 - \cos\frac{2\pi s}{N}\right)\right], \quad -\infty < t < \infty \tag{16}$$

with $H(t)$ the Heaviside step function

$$H(t) = \begin{cases} 1 & \text{if} \quad t > 0 \\ \frac{1}{2} & \text{if} \quad t = 0 \\ 0 & \text{if} \quad t < 0 \end{cases} \tag{17}$$

[with the property $\partial H/\partial t = \delta(t)$] satisfies a discrete Green's function equation analogous to (10). Let us take the derivative with respect to t:

$$\begin{aligned}\frac{dp_0(l, t)}{dt} &= \delta(t)N^{-1}\sum_{s=1}^{N}\exp\frac{2\pi i s l}{N} \\ &\quad + \alpha H(t)N^{-1}\sum_{s=1}^{N}\left\{\left(\exp\frac{2\pi i(l + 1)s}{N} - 2 + \exp\frac{-2\pi i(l - 1)s}{N}\right)\right. \\ &\quad \times \left.\exp\left[-2\alpha\tau\left(1 - \cos\frac{2\pi s}{N}\right)\right]\right\}\end{aligned} \tag{18}$$

so that

$$\frac{dp_0(l, t)}{dt} - \alpha[p_0(l + 1, t) - 2p_0(l, t) + p_0(l - 1, t)] = \delta(t)\delta_{l,0} \tag{19}$$

This is a well-known differential equation which is encountered in the theory of random walks on a line in which equal probabilities exist for a step to either the right or the left of one lattice spacing in a short time.[5]

The discrete quantum analog of (16) is

$$K_0(l, t) = H(t)N^{-1}\sum_{s=1}^{N}\exp\{(2\pi i l s/N) - 2i\alpha t[1 - \cos(2\pi s/N)]\} \tag{20}$$

which satisfies

$$i\frac{dK_0(l, t)}{dt} + \alpha[K_0(l + 1, t) - 2K_0(l, t) + K_0(l - 1, t)] = i\delta(t)\delta_{l,0} \tag{21}$$

It also can be shown to satisfy the unitarity equation

$$\sum_{l=1}^{N} K_0(l - l_0, t)K_0^*(l - l_1, t) = \delta_{l_0 l_1} \tag{22}$$

when $t > 0$. Direct substitution into the left-hand side of this equation yields

$$N^{-2} \sum_{l=1}^{N} \sum_{s_1=1}^{N} \sum_{s_2=1}^{N} \exp\{2\pi i[(l - l_0)s_1 - (l - l_1)s_2]/N\}$$
$$\times \exp\{2i\alpha t[\cos(2\pi s_1/N) - \cos(2\pi s_2/N)]$$

$$= N^{-1} \sum_{s_1=1}^{N} \sum_{s_2=1}^{N} \delta_{s_1,s_2} \exp[2\pi i(l_1 s_2 - l_0 s_1)/N]$$
$$\times \exp\{2i\alpha t[\cos(2\pi s_1/N) - \cos(2\pi s_2/N)]$$
$$= N^{-1} \sum_{s=1}^{N} \exp[2\pi i(l_1 - l_0)s/N] = \delta_{l_1,l_0}$$

as required.

Equation (21) reduces to the free particle Schrödinger equation when $\alpha = \hbar/2ma^2$, with a a lattice spacing and $K_0(l, t)$ interpreted to be the propagator at the point $x = la$. As $a \to 0$, (21) becomes (11).

The three dimensional analog of (13) on a simple cubic lattice is [with positions being identified by (l_1, l_2, l_3)]

$$p_0(l, t) = (1/N^3) \sum_{s_1 s_2 s_3=1}^{N} \exp\{(2\pi i l \cdot s/N) - 2\alpha t[3 - (c_1 + c_2 + c_3)]\} \tag{23}$$

with

$$c_j \equiv \cos(2\pi s_j/N) \qquad \text{and} \qquad l \cdot s = l_1 s_1 + l_2 s_2 + l_3 s_3 \tag{24}$$

Similarly the analog of (20) is

$$K_0(l, t) = (1/N^3) \sum_{s_1 s_2 s_3=1}^{N} \exp\{(2\pi i l \cdot s/N) - 2i\alpha t[3 - (c_1 + c_2 + c_3)]\} \tag{25}$$

In the limit as the number of lattice points $N \to \infty$, the transition probability (16) becomes (setting $\theta = 2\pi s/N$, $d\theta = 2\pi/N$)

$$p_0(l, t) = (1/2\pi)H(t) \int_0^{2\pi} e^{il\theta} e^{-2\alpha t(1-\cos\theta)}\, d\theta$$
$$= H(t)e^{-2\alpha t} I_l(2\alpha t) \tag{26}$$

Similarly the one-dimensional propagator (20) becomes

$$K_0(l, t) = H(t)e^{-2\alpha i t} J_l(2\alpha t) \tag{27}$$

where J_l is the lth Bessel function and I_l is the lth Bessel function of purely imaginary argument. The propagator for a 3D simple cubic lattice is

$$K_0(l, t) = H(t)J_{l_1}(2\alpha t)J_{l_2}(2\alpha t)J_{l_3}(2\alpha t)e^{-6i\alpha t} \tag{28}$$

Our propagator $K(l, t)$ describes the manner in which our system responds to a transient point source at the origin at time $t = 0$. From its definition, the response to distributed sources which are continually operative is

$$\psi(l, t) = \sum_{l_0} \int_{-\infty}^{t} K(l - l_0, t - \tau)\psi_0(l_0, \tau)\, d\tau \tag{29}$$

3. ON THE EFFECT OF THE INTRODUCTION OF TRAPS ON A LATTICE

Again let us start with a consideration of a random walker in the neighborhood of a trap from which he cannot escape. The general rate equation for a Markovian process of which our random walk is an example is[8]

$$dP_l(t)/dt = \sum_m p_{lm}P_m(t) - \sum_m p_{ml}P_l(t) \tag{30}$$

The constants p_{lm} represent probabilities per unit time of transitions from state m to l if a system is already in m. Hence the usual interpretation given to the positive term on the right-hand side of (30) is that it gives the rate at which transitions are made into state l, while the negative term represents the rate of transitions out of state l. Hence, if a state l_1 is a trap, no transitions from l_1 to any other l occurs and we must set $p_{l,l_1} = 0$ for $l \neq l_1$, so that generally we replace $p_{l,m}$ by $p_{l,m}(1 - \delta_{m,l_1})$ for all l and m and Eq. (30) would be changed to read

$$\frac{dP_l(t)}{dt} - \sum_m p_{l,m}P_m(t) + \sum_m p_{ml}P_l(t) = -\sum_m p_{lm}\delta_{m,l_1}P_m(t) + \sum_m p_{ml}\delta_{l,l_1}P_l(t) \tag{31}$$

The random walk model characterized by Eq. (19) in the last section is of the form (30) with

$$p_{l,m} = \alpha(\delta_{l-m,1} - 2\delta_{l-m,0} + \delta_{l-m,-1})$$

Hence with a trap at $l = l_1$, (19) becomes

$$\frac{dp(l, t)}{dt} - \alpha[p(l + 1, t) - 2p(l, t) + p(l - 1, t)] = \delta(t)\delta_{l,0} - \alpha[\delta_{l-l_1,1} - 2\delta_{l,l_1} + \delta_{l-l_1,-1}]p(l_1, t)$$

The various coefficients of $K_0(m)$ in Eq. (21) with $m = l, l \pm 1$ represent transition amplitudes into and out of various lattice points. Hence, if lattice point l_1 is a trap, all transition amplitudes for transitions out of the trap are zero so that the same line of reasoning that was applied to the derivation of the above equation applies to its quantum analog:

$$\frac{dK(l, t)}{dt} - i\alpha[K(l + 1, t) - 2K(l, t) + K(l - 1, t)]$$
$$= \delta(t)\delta_{l,0} - i\alpha(\delta_{l,l_1+1} - 2\delta_{l,l_1} + \delta_{l,l_1-1})K(l_1, t) \tag{32}$$

The Laplace transform of (32) can be taken, recalling that

$$\int_0^\infty \frac{dK(l, t)}{dt} e^{-ut}\, dt = -K(l, 0) + u \int_0^\infty e^{-ut}K(l, t)\, dt$$
$$= uK(l, u) - \tfrac{1}{2}\delta_{l,0} \tag{33}$$

The propagator $K(l, t)$ can be interpreted to represent the development of an instantaneous point source pulse generated at the origin at time $t = 0$. The evolution of an initially dispersed source, which can be characterized by a wave function $\psi(l, 0)$, is given by

$$\psi(l, t) = \sum_{l'} K(l - l', t)\psi(l', 0)$$

We define $K(l, u)$ to be the Laplace transform of $K(l, t)$. Then

$$uK(l, u) - i\alpha[K(l + 1, u) - 2K(l, u) + K(l - 1, u)]$$
$$= \delta_{l,0} - i\alpha K(l_1, u)[\delta_{l,l_1+1} - 2\delta_{l,l_1} + \delta_{l,l_1-1}] \tag{34}$$

We have used the equation

$$\int_0^\infty \delta(t)e^{-\alpha t}\, dt = \tfrac{1}{2} \tag{35}$$

In a similar way it can be shown that the unperturbed propagator equation (32) has the Green's function form

$$uK_0(l, u) - i\alpha[K_0(l + 1, u) - 2K_0(l, u) + K_0(l - 1, u)] = \delta_{l,0} \tag{36}$$

It can easily be verified that

$$K(l, u) = \sum_{l'} \{\delta_{l',0} - i\alpha K(l_1, u)[\delta_{l',l_1+1} - 2\delta_{l',l_1} + \delta_{l',l_1-1}]\}K_0(l - l', u)$$
$$= K_0(l, u) - i\alpha K(l_1, u)$$
$$\times [K_0(l - l_1 - 1, u) - 2K_0(l - l_1, u) + K_0(l - l_1 + 1, u)]$$
$$= K_0(l, u) - [uK_0(l - l_1, u) - \delta_{l,l_1}]K(l_1, u) \tag{37}$$

Now set $l = l_1$. Then

$$K(l_1, u) = K_0(l_1, u)/uK_0(0, u) \tag{38}$$

When this is substituted into (37) it is found that

$$K(l, u) = \begin{cases} \dfrac{K_0(l, u)K_0(0, u) - K_0(l - l_1, u)K_0(l_1, u)}{K_0(0, u)} & \text{if} \quad l \neq l_1 \\ K_0(l_1, u)/uK_0(0, u) & \text{if} \quad l = l_1 \end{cases} \tag{39}$$

The first term in (39) (when $l \neq l_1$) corresponds to the propagator in the absence of traps, while the second (negative) term corresponds to all paths that go through the trap. The difference then represents all paths that start at the origin and end at l without going through l_1, The time-dependent propagator $K(l, t)$ is obtained from (39) by taking the inverse Laplace transform.

The effect of a trap on the propagation of a plane wave can be discussed in a similar way. We search first for a solution of (21) that, in the absence of a trap, would correspond to a plane wave propagating in our lattice. Suppose that

$$\psi_0(l, t) = \exp -i(\omega t - kl) \tag{40}$$

Since $\psi_0(l, t)$ satisfies (21) with the delta function omitted, a dispersion relation exists between $\omega(k)$ and k

$$\omega(k) = 2\alpha(1 - \cos k) \tag{41}$$

In the presence of a trap our basic wave equation is [see (32) without the delta function on the right-hand side]

$$\frac{d\psi(l, t)}{dt} - i\alpha[\psi(l + 1, t) - 2\psi(l, t) + \psi(l - 1, t)]$$
$$= -i\alpha(\delta_{l,l_1+1} - 2\delta_{l,l_1} + \delta_{l,l_1-1})\psi(l_1, t) \tag{42}$$

We search for a solution of the form

$$\psi(l, t) = e^{-i\omega t}\{e^{ikl} + F(l)\} \tag{43}$$

When (43) is substituted into (42) we obtain the following equation for $F(l)$ [after using (41)]

$$\omega F(l) + \alpha[F(l + 1) - 2F(l) + F(l - 1)]$$
$$= \alpha[\exp(ikl_1) + F(l_1)](\delta_{l,l_1+1} - 2\delta_{l,l_1} + \delta_{l,l_1-1}) \tag{44}$$

Let us define $F_0(l) \equiv F_0(l, \omega)$ to be the Green's function that satisfies

$$\omega F_0(l, \omega) + \alpha[F_0(l + 1, \omega) - 2F_0(l, \omega) + F_0(l - 1, \delta)] = \delta_{l,0} \tag{45}$$

As is usual in scattering theory, this Green's function should represent an outgoing wave propagating in both directions away from the origin. It is clear that $F_0(l)\exp(-i\omega t)$, with

$$F_0(l) = [2i\alpha \sin k]^{-1} \exp(ik|l|) \tag{46}$$

has this property, while $F_0(l)$ is a solution of (45).

The standard formula for solving an inhomogeneous linear equation in terms of the Green's function of the homogeneous equation can be applied to (44) to yield

$$\begin{aligned} F(l, \omega) &= \alpha \sum_{l'} [F(l_1, \omega) + \exp(ikl_1)] \\ &\quad \times (\delta_{l',l_1+1} - 2\delta_{l',l_1} + \delta_{l',l_1-1}) F_0(l - l', \omega) \end{aligned} \tag{47}$$

the right-hand side of (44) being the "inhomogeneous term." Hence

$$\begin{aligned} F(l) &= [F(l_1) + \exp(ikl_1)] \\ &\quad \times \alpha[F_0(l - l_1 - 1) - 2F_0(l - l_1) + F_0(l - l_1 + 1)] \end{aligned} \tag{48}$$

which, in view of (45) becomes

$$F(l) = \{F(l_1) + \exp(ikl_1)\}\{\delta_{l,l_1} - \omega F_0(l - l_1)\} \tag{49}$$

If we let $l = l_1$, we can find the unknown quantity $F(l_1)$ on the right-hand side of (49). Then

$$F(l_1) + \exp(ikl_1) = \{\exp(ikl_1)\}/\omega F_0(0)$$

so that (43) and (49) yield

$$\psi(l, t) = e^{-i\omega t} \begin{cases} e^{ikl} - e^{ikl_1} F_0(l - l_1)/F_0(0) & \text{if} \quad l \neq l_1 \\ e^{ikl_1}/\omega F_0(0) & \text{if} \quad l = l_1 \end{cases} \tag{50}$$

We can verify that our model of a trap truly behaves like a trap by substituting (46) into (50) and considering the final formula for $\psi(l, t)$ when $l \neq l_1$

$$\begin{aligned} \psi(l, t) &= \{\exp[-i(\omega t - kl)]\}\{1 - \exp[ik(l_1 - l)]\exp(ik|l_1 - l|)\} \\ &= \begin{cases} 0 & \text{if} \quad l > l_1 \\ \{\exp[-i(\omega t - kl)]\}\{1 - \exp[-2ik(l - l_1)]\} & \text{if} \quad l < l_1 \end{cases} \end{aligned} \tag{51}$$

Hence $|\psi(l, t)|^2 = 0$, if $l > l_1$, so that, as required, no wave passes the trap.

Let us now consider the case of two traps on a two-dimensional lattice, first investigating their influence on a point source disturbance and then on a plane wave. The unperturbed 2D equation analogous to (21) is, for lattice point (l, m),

$$i\frac{dK_0(l, m; t)}{dt} + \alpha\, \Delta^2 K_0(l, m; t) = i\, \delta(t)\delta_{l,0}\delta_{m,0} \tag{52}$$

where

$$\Delta^2 f(l, m) = f(l+1, m) - 2f(l, m) + f(l-1, m) + f(l, m+1) - 2f(l, m) + f(l, m-1) \tag{53}$$

If we follow the derivation of (32), we find that when there are two defects, one at $l_1 \equiv (l_1, m_1)$ and the other at $l_2 \equiv (l_2, m_2)$,

$$\frac{dK(l, m;t)}{dt} - i\alpha\, \Delta^2 K(l, m;t) = \delta(t)\delta_{l,0}\delta_{m,0} - i\alpha \sum_{\beta=1}^{2} K(l_\beta, m_\beta;t)\, \Delta_\beta{}^2(\delta_{l,l_\beta}\delta_{m,m_\beta}) \tag{54}$$

where the subscript β on $\Delta_\beta{}^2$ implies that the operator acts on (l_β, m_β) and not on the (l, m). Upon the taking of Laplace transforms and the introduction of the Green's function $K_0(l, m;u)$ of the Laplace transform of $K_0(l, m;t)$, with $K_0(l, m; t)$ being the solution of

$$uK_0(l, m; u) - i\alpha\, \Delta^2 K_0(l, m; u) = \delta_{l,0}\delta_{m,0} \tag{55}$$

we find the Laplace transform $K(l, m; u) \equiv K(l, m)$ to be given by [following (37)]

$$\begin{aligned} K(l, m) &= \sum_{l'm'} \{\delta_{l',0}\delta_{m',0} - \sum_{\beta=1}^{2} i\alpha K(l_\beta, m_\beta)\, \Delta_\beta{}^2\delta_{l',l_\beta}\delta_{m'm_\beta}\} \\ &\quad \times K_0(l - l', m - m') \\ &= K_0(l, m) - i\alpha \sum_{\beta=1}^{2} K(l_\beta, m_\beta)\, \Delta_\beta{}^2 K_0(l - l_\beta, m - m_\beta) \end{aligned} \tag{56}$$

We now abbreviate $\boldsymbol{l} \equiv (l, m)$ and $f(l, m) \equiv f(\boldsymbol{l})$ and employ the definition (55) of $K_0(\boldsymbol{l}) \equiv K_0(l, m)$. Then (56) reduces to

$$K(\boldsymbol{l}, u) = K_0(\boldsymbol{l}, u) + \sum_{\beta=1}^{2} K(\boldsymbol{l}_\beta, u)\{\delta_{\boldsymbol{l}-\boldsymbol{l}_\beta,0} - uK_0(\boldsymbol{l} - \boldsymbol{l}_\beta, u)\} \tag{57}$$

which, incidentally, applies to n defects if the upper limit 2 on the β summation is replaced by n. Equation (57) is clearly applicable to a 3D simple cubic lattice, if the vector $\boldsymbol{l}$ is given a third component. When we know the propagator K_0, we will have a closed expression for $K(l, u)$ which contains only known functions.

Let us successively let $\boldsymbol{l}$ in (57) be $\boldsymbol{l}_1$ and $\boldsymbol{l}_2$. Then we obtain the pair of inhomogeneous equations for $K(\boldsymbol{l}_1, u)$ and $K(\boldsymbol{l}_2, u)$

$$\begin{aligned} uK_0(0, u)K(\boldsymbol{l}_1, u) + uK_0(\boldsymbol{l}_1 - \boldsymbol{l}_2, u)K(\boldsymbol{l}_2, u) &= K_0(\boldsymbol{l}_1, u) \\ uK_0(\boldsymbol{l}_2 - \boldsymbol{l}_1, u)K(\boldsymbol{l}_1, u) + uK_0(0, u)K(\boldsymbol{l}_2, u) &= K_0(\boldsymbol{l}_2, u) \end{aligned} \tag{58}$$

Then, if

$$\Delta_2 = \begin{vmatrix} K_0(0, u) & K_0(l_1 - l_2, u) \\ K_0(l_2 - l_1, u) & K_0(0, u) \end{vmatrix} \tag{59a}$$

$$uK(l_1, u) = \frac{1}{\Delta_2} \begin{vmatrix} K_0(l_1, u) & K_0(l_1 - l_2, u) \\ K_0(l_2, u) & K_0(0, u) \end{vmatrix} \tag{59b}$$

$$uK(l_2, u) = -\frac{1}{\Delta_2} \begin{vmatrix} K_0(l_1, u) & K_0(0, u) \\ K_0(l_2, u) & K_0(l_2 - l_1, u) \end{vmatrix} \tag{59c}$$

If (59) is substituted into (57), it is found that if $l \neq l_1$ or l_2 and if the origin of the walk is l_0 rather than 0, then ($\mathscr{L}^{-1}$ being the inverse Laplace transform operator)

$$K(l - l_0, t) = \mathscr{L}^{-1} \frac{\begin{vmatrix} K_0(l - l_0, u) & K_0(l - l_1, u) & K_0(l - l_2, u) \\ K_0(l_1 - l_0, u) & K_0(0, u) & K_0(l_1 - l_2, u) \\ K_0(l_1 - l_0, u) & K_0(l_2 - l_1, u) & K_0(0, u) \end{vmatrix}}{\begin{vmatrix} K_0(0, u) & K_0(l_1 - l_2, u) \\ K_0(l_2 - l_1, u) & K_0(0, u) \end{vmatrix}} \tag{59d}$$

An expansion of the determinants yields terms which can be identified with the diagrams indicated in Fig. 1.

We proceed in essentially the same way to discuss the scattering of a plane wave by two traps. Our basic equation for the wave function $\psi(l, t)$ is

$$d\psi(l, t)/dt - i\alpha\, \Delta^2\psi(l, t) = -i\alpha \sum_{\beta=1}^{2} \psi(l_\beta)\, \Delta_\beta{}^2 \delta_{l, l_\beta} \tag{60}$$

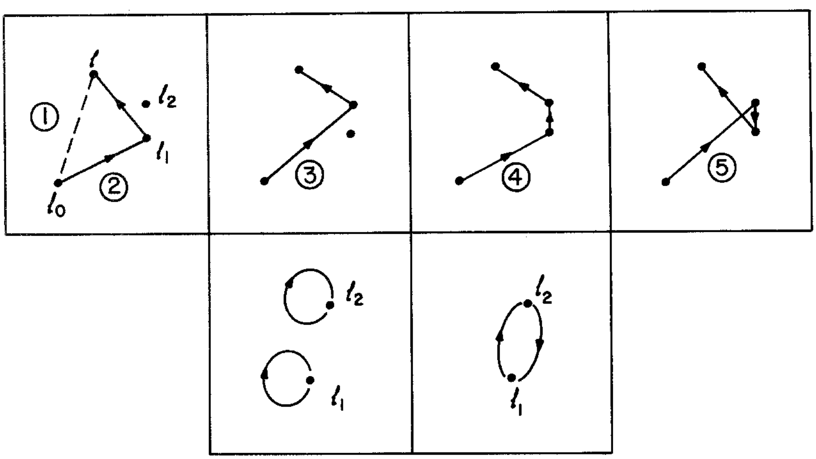

Fig. 1. The diagrammatic interpretation of all the terms which appear in the scattering of a pulse by two absorbing centers.

Let us assume that if in the absence of traps our wave function is the plane wave

$$\psi_0(\boldsymbol{l}, t) = \exp -i(\omega t - \mathbf{k}\cdot\boldsymbol{l}) \tag{61a}$$

with the dispersion relation (on a 3D simple cubic lattice)

$$\omega = 2\alpha(3 - \cos k_1 - \cos k_2 - \cos k_3) \tag{61b}$$

then in the presence of traps it becomes

$$\psi(\boldsymbol{l}, t) = [\exp(-i\omega t)]\{\exp(i\mathbf{k}\cdot\boldsymbol{l}) + F(\boldsymbol{l})\} \equiv [\exp(-i\omega t)]\psi(\boldsymbol{l}) \tag{62}$$

When (62) is substituted into (60) we find that

$$\omega F(\boldsymbol{l}) + \alpha\,\Delta^2 F(\boldsymbol{l}) = \alpha \sum_{\beta=1}^{2} [F(\boldsymbol{l}_\beta) + \exp(i\mathbf{k}\cdot\boldsymbol{l})]\,\Delta_\beta{}^2\delta_{\boldsymbol{l},\boldsymbol{l}_\beta} \tag{63}$$

As usual, if we let $F_0(\boldsymbol{l})$ be the Green's function solution of

$$\omega F_0(\boldsymbol{l}) + \alpha\,\Delta^2 F_0(\boldsymbol{l}) = \delta_{\boldsymbol{l},0} \tag{64}$$

then

$$\begin{aligned} F(\boldsymbol{l}) &= \alpha \sum_{\boldsymbol{l}} \sum_{\beta=1}^{2} [F(\boldsymbol{l}_\beta) + \exp(i\mathbf{k}\cdot\boldsymbol{l}_\beta]F_0(\boldsymbol{l} - \boldsymbol{l}_\beta)\Delta_\beta{}^2\delta_{\boldsymbol{l},\boldsymbol{l}_\beta} \\ &= \alpha \sum_{\beta=1}^{2} [F(\boldsymbol{l}_\beta) + \exp(i\mathbf{k}\cdot\boldsymbol{l}_\beta]\,\Delta_\beta{}^2 F_0(\boldsymbol{l} - \boldsymbol{l}_\beta) \end{aligned} \tag{65}$$

However, in view of (62) and noting that

$$\alpha\,\Delta_\beta{}^2 F_0(\boldsymbol{l} - \boldsymbol{l}_\beta) = \delta_{\boldsymbol{l},\boldsymbol{l}_\beta} - \omega F_0(\boldsymbol{l} - \boldsymbol{l}_\beta)$$

we have

$$\psi(\boldsymbol{l}) = \exp(i\mathbf{k}\cdot\boldsymbol{l}) + \sum_{\beta=1}^{2} \psi(\boldsymbol{l}_\beta)\{\delta_{\boldsymbol{l},\boldsymbol{l}_\beta} - \omega F_0(\boldsymbol{l} - \boldsymbol{l}_\beta)\} \tag{66}$$

If $\boldsymbol{l} \neq \boldsymbol{l}_1, \boldsymbol{l}_2$, then

$$\psi(\boldsymbol{l}) = \exp(i\mathbf{k}\cdot\boldsymbol{l}) - \sum_{\beta} \psi(\boldsymbol{l}_\beta)F_0(\boldsymbol{l} - \boldsymbol{l}_\beta) \tag{67}$$

Now let $\boldsymbol{l}$ be successively $\boldsymbol{l}_1$ and $\boldsymbol{l}_2$ in Eq. (67). The two resulting equations can be solved for $\psi(\boldsymbol{l}_1)$ and $\psi(\boldsymbol{l}_2)$. When these results are substituted into (67) the final expression obtained for $\psi(\boldsymbol{l})$ is, for $\boldsymbol{l} \neq \boldsymbol{l}_1, \boldsymbol{l}_2$,

$$\psi(\boldsymbol{l}) = \frac{\begin{vmatrix} \exp i\mathbf{k}\cdot\boldsymbol{l} & F_0(\boldsymbol{l} - \boldsymbol{l}_1, \omega) & F_0(\boldsymbol{l} - \boldsymbol{l}_2, \omega) \\ \exp i\mathbf{k}\cdot\boldsymbol{l}_1 & F_0(0, \omega) & F_0(\boldsymbol{l}_1 - \boldsymbol{l}_2, \omega) \\ \exp i\mathbf{k}\cdot\boldsymbol{l}_2 & F_0(\boldsymbol{l}_2 - \boldsymbol{l}_1, \omega) & F_0(0, \omega) \end{vmatrix}}{\begin{vmatrix} F_0(0, \omega) & F_0(\boldsymbol{l}_1 - \boldsymbol{l}_2, \omega) \\ F_0(\boldsymbol{l}_2 - \boldsymbol{l}_1, \omega) & F_0(0, \omega) \end{vmatrix}} \tag{68}$$

The structure of this determinant is clearly very similar to (59d).

In the case of n isolated, perfectly absorbing traps our basic propagation equations are (57) and (67) with the upper limit 2 on the β summation replace by n. Then, if we successively let $\boldsymbol{l} = \boldsymbol{l}_1, \boldsymbol{l}_2,..., \boldsymbol{l}_n$, we obtain n linear equations analogous to (58). These equations for either $K(\boldsymbol{l}_j, u)$ or $\psi(\boldsymbol{l}_j)$ have solutions, which are ratios of determinants. When these are substituted into the generalization of (57) or (67) we obtain an object of the form

$$W(l) = D_n/\Delta_n \tag{69}$$

where

$$D_n = \det k_{\alpha\beta} \qquad \text{with} \quad \alpha, \beta = 0, 1, 2,... \tag{70a}$$

and n is a similar determinant with the left column and top row reversed

$$\Delta_n = \det k_{\alpha\beta} \qquad \text{with} \quad \alpha, \beta = 1, 2,..., n \tag{70b}$$

The $W(l)$ and $k_{\alpha\beta}$ have the following form for the point source scattering problem:

$$W(l) \equiv K(\boldsymbol{l} - \boldsymbol{l}_0, u), \qquad k_{00} \equiv K_0(\boldsymbol{l} - \boldsymbol{l}_0, u) \tag{71a}$$

$$k_{0\beta} \equiv K_0(\boldsymbol{l} - \boldsymbol{l}_\beta, u), \qquad k_{\beta 0} \equiv K_0(\boldsymbol{l}_\beta - \boldsymbol{l}_0, u), \qquad \beta > 0 \tag{71b}$$

$$k_{\alpha\beta} = K(\boldsymbol{l}_\alpha - \boldsymbol{l}_\beta, u), \qquad \alpha, \beta = 1,2,..., n \tag{71c}$$

For the scattering of a plane wave the $W(l)$ and $k_{\alpha\beta}$ are

$$W(l) \equiv \psi(\boldsymbol{l}), \qquad k_{00} \equiv \exp(i\mathbf{k}\cdot\boldsymbol{l}) \tag{72a}$$

$$k_{\alpha\beta} \equiv F_0(\boldsymbol{l} - \boldsymbol{l}_\beta, \omega), \qquad k_{\beta 0} \equiv \exp(i\mathbf{k}\cdot\boldsymbol{l}_\beta), \qquad \beta > 0 \tag{72b}$$

$$k_{\alpha\beta} \equiv F_0(\boldsymbol{l}_\alpha - \boldsymbol{l}_\beta, \omega), \qquad \alpha, \beta > 0 \tag{72c}$$

The resulting generalization of (68) given by (69) with the above definitions of terms represents all possible ways energy in the bear incident on the traps can be depleted by trapping before it propagates away from the traps. While the solution of the scattering problem has been reduced to quadratures, numerical estimates of depletion and scattering depend on calculations of the lattice Green's functions $F_0(\boldsymbol{l}, \omega)$. Those functions are discussed in detail in Section 5.

4. ON THE EFFECT OF ABNORMAL BONDS IN THE LATTICE MODEL

A more general type of abnormality will now be considered and analyzed in the same manner in which we analyzed the effect of traps. The medium described by our basic model equation (21) is characterized by the parameter α. If the medium is not homogeneous it may suffer inhomogeneities (which become scattering centers) in the way in which one lattice point is connected to another. A one-dimensional inhomogeneous chain might be characterized by a set of numbers $\alpha_{l+1,l}$ such that the basic equation for the irregular system would have the form

$$i\frac{dK(l,t)}{dt} + \alpha_{l+1,l}[K(l+1,t) - K(l,t)] - \alpha_{l,l-1}[K(l,t) - K(l-1,t)] = i\,\delta(t)\delta_{l,0} \tag{73}$$

which would reduce to (21) if $\alpha_{l+1,l} \equiv \alpha$ for all l. An alternative form for (73) is

$$\begin{aligned}\frac{dK(l,t)}{dt} &- i\alpha[K(l+1,t) - 2K(l,t) + K(l-1,t)] \\ &= i\alpha\{\epsilon_{l+1,l}[K(l+1,t) - K(l,t)] \\ &\quad - \epsilon_{l,l-1}[K(l,t) - K(l-1,t)]\} + \delta(t)\delta_{l,0}\end{aligned} \tag{74}$$

where

$$\epsilon_{l+1,l} \equiv (\alpha_{l+1,l} - \alpha)/\alpha \tag{75}$$

and the right-hand side of (74) can be considered to contain the influence of a scattering potential. We again start our discussion with an investigation of the propagation of an instantaneous pulse source initially at the origin.

As in Section 3 we take Laplace transforms and define $K_0(l, u)$ by (36). It is the Green's function associated with a perfect lattice model. Then $K(l, u)$ can be expressed in terms of $K_0(l, u)$ in a manner analogous to that discussed in Section 3. The analog of (37) is [with $K(l) \equiv K(l, u)$]

$$\begin{aligned}K(l,u) &= \sum_{l'}\{\delta_{l',0} + \alpha i\epsilon_{l'+1,l'}[K(l'+1) - K(l')] \\ &\qquad - i\alpha\epsilon_{l',l'-1}[K(l') - K(l'-1)]\}K_0(l-l') \\ &= K_0(l,u) + i\sum_{l'}\alpha\epsilon_{l'+1,l'}[K(l'+1) - K(l')] \qquad (76a)\\ &\qquad \times [K_0(l-l') - K_0(l-l'-1)] \\ &= K_0(l,u) + i\sum_{l'}\alpha\epsilon_{l'+1,l'}P(l,u)P_0(l-l'-1,u) \qquad (76b)\end{aligned}$$

where we define

$$P(l,u) \equiv K(l+1,u) - K(l,u) \tag{77}$$

An equation can also be found for $P(l, u)$. From (76a)

$$\begin{aligned}P(l,u) &= P_0(l,u) + i\sum_{l'}\alpha\epsilon_{l'+1,l'}P(l',u) \\ &\qquad \times [K_0(l-l'+1,u) - 2K_0(l-l',u) + K_0(l-l'-1,u)] \\ &= P_0(l,u) + \sum_{l'}\epsilon_{l'+1,l'}P(l,u)[uK_0(l-l',u) - \delta_{l',l}]\end{aligned} \tag{78}$$

Let us first consider the case of two "defective" bonds, i.e.,

$$\epsilon_{l'+1,l'} \equiv \delta_{l',l_1}\epsilon_1 + \delta_{l',l_1}\epsilon_2 \tag{79}$$

and successively let l in Eq. (78) be l_1 and l_2. Then, if we also let

$$\alpha_j = 1 + \epsilon_j$$

we have

$$-P_0(l_1) = P(l_1)[u\epsilon_1 K_0(0) - \alpha_1] + P(l_2)u\epsilon_2 K_0(l_1 - l_2) \tag{80a}$$

$$-P_0(l_2) = P(l_1)u\epsilon_1 K_0(l_2 - l_1) + P(l_2)[u\epsilon_2 K_0(0) - \alpha_2] \tag{80b}$$

If we solve for $P(l_1) \equiv P((l_1, u)$ and $P(l_2)$ and substitute the resulting expressions into (76b) when l' runs through l_1 and l_2, we find

$$K(l, u) = \Delta_2^{-1} \begin{vmatrix} K_0(l) & P_0(l_1) & P_0(l_2) \\ i\alpha\epsilon_1 P_0(l - l_1 - 1) & u\epsilon_1 K_0(0) - \alpha_1 & u\epsilon_1 K_0(l_2 - l_1) \\ i\alpha\epsilon_2 P_0(l - l_2 - 1) & u\epsilon_2 K_0(l_1 - l_2) & u\epsilon_1 K_0(0) - \alpha_2 \end{vmatrix} \tag{81a}$$

with

$$\Delta_2 = \begin{vmatrix} u\epsilon_1 K_0(0) - \alpha_1 & u\epsilon_1 K_0(l_2 - l_1) \\ u\epsilon_2 K_0(l_1 - l_2) & u\epsilon_2 K_0(0) - \alpha_2 \end{vmatrix} \tag{81b}$$

One can easily combine the methods of the last section with the model discussed above to find the wave function of a plain wave scattered by our pair of abnormal bonds characterized by (79). If the incident wave function in the absence of the scatterer is

$$\psi_0(l, t) = \exp -i(\omega t - kl) \tag{82}$$

then that of the wave function in presence of the scatterer becomes

$$\psi(l, t) = \psi(l) \exp - i\omega t$$

with

$$\psi(l) = \Delta_2^{-1} \begin{vmatrix} e^{ik\cdot l} & (i - e^{ik})e^{ikl_1} & (i - e^{ik})e^{ikl_2} \\ \alpha\epsilon_1 Q_0(l - l_1 - 1) & \omega\epsilon_1 F_0(0) - \alpha_1 & \omega\epsilon_1 F_0(l_2 - l_1) \\ \alpha\epsilon_2 Q_0(l - l_2 - 1) & \omega\epsilon_2 F_0(l_1 - l_2) & \omega\epsilon_2 F_0(0) - \alpha_2 \end{vmatrix} \tag{83a}$$

We have used the abbreviations

$$\Delta_2 = \begin{vmatrix} \omega\epsilon_1 F_0(0) - \alpha_1 & \omega\epsilon_1 F_0(l_2 - l_1) \\ \omega\epsilon_2 F_0(l_1 - l_2) & \omega\epsilon_2 F_2(0) - \alpha_2 \end{vmatrix} \tag{83b}$$

$$Q_0(l) = F_0(l + 1) - F_0(l) \tag{83c}$$

and from (46)

$$F_0(l) = (2i\alpha \sin k)^{-1} \exp(ik|l|) \tag{83d}$$

The similarity of (83a) to (81a) is clear.

These results can be extended easily to two- and three-dimensional lattices and to n unusual bonds. Since the equations are slightly shorter in the 2D case than in the 3D case, we will consider that case first and since the generalization from two to three dimensions will be obvious, we will merely exhibit final 3D formulas. If we define a typical lattice point on a 2D lattice to be $\mathbf{l} \equiv (l, m)$, then the basic equation analogous to (74) for a point source excitation is

$$dK(\mathbf{l})/dt - i\alpha\,\Delta^2 K(\mathbf{l}) - \delta(t)\delta_{l,0}\delta_{m,0}$$
$$= i\alpha\{\epsilon(\mathbf{l}+\mathbf{i},\mathbf{l})[K(\mathbf{l}+\mathbf{i}) - K(\mathbf{l})] - \epsilon(\mathbf{l}-\mathbf{i})[K(\mathbf{l}) - K(\mathbf{l}-\mathbf{i})]$$
$$+ \epsilon(\mathbf{l}+\mathbf{j},\mathbf{l})[K(\mathbf{l}+\mathbf{j}) - K(\mathbf{l})] - \epsilon(\mathbf{l}-\mathbf{j})[K(\mathbf{l}) - K(\mathbf{l}-\mathbf{j})]\} \qquad (84)$$

where

$$\mathbf{l} \equiv (l, m), \qquad \mathbf{i} \equiv (1, 0), \qquad \mathbf{j} \equiv (0, 1), \qquad \mathbf{l}+\mathbf{i} \equiv (l+1, m), \qquad \text{etc.}$$

and the ϵ's are defined to be

$$\epsilon(\mathbf{l}+\mathbf{i},\mathbf{l}) = \{\alpha(\mathbf{l}+\mathbf{i},\mathbf{l}) - \alpha\}/\alpha \qquad (85)$$

$$\epsilon(\mathbf{l}+\mathbf{j},\mathbf{l}) = \{\alpha(\mathbf{l}+\mathbf{j},\mathbf{l}) - \alpha\}/\alpha \qquad (86)$$

the first being associated with the deviation from α of the bond parameter associated with the horizontal bond connecting $(l+1, m)$ to (l, m). The second is a typical deviation associated with an unusual vertical bond.

The 2D generalization of Eq. (76b) is

$$K(\mathbf{l}) = K_0(\mathbf{l}) + i\alpha \sum_{\mathbf{l}'} \{\epsilon(\mathbf{l}'+\mathbf{i},\mathbf{l}')G^1(\mathbf{l}')G_0(\mathbf{l}-\mathbf{l}'-\mathbf{i})$$
$$+ \epsilon(\mathbf{l}'+\mathbf{j},\mathbf{l}')G^2(\mathbf{l}')G_0{}^2(\mathbf{l}-\mathbf{l}'-\mathbf{j})\} \qquad (87)$$

where we have now to define two functions analogous to the $P(\mathbf{l}, u)$ of (77). They are

$$G^1(\mathbf{l}) \equiv K(\mathbf{l}+\mathbf{i}, u) - K(\mathbf{l}, u) \qquad (88a)$$

$$G^2(\mathbf{l}) \equiv K(\mathbf{l}+\mathbf{j}, u) - K(\mathbf{l}, u) \qquad (88b)$$

the first being associated with the horizontal bond connecting $(l+1, m)$ to (l, m) and the second with the vertical bond connecting $(l, m+1)$ to (l, m). Our final formulas will be considerably condensed if we introduce a matrix

$$F(\mathbf{l}) = \begin{vmatrix} F_{11}(\mathbf{l}) & F_{12}(\mathbf{l}) \\ F_{21}(\mathbf{l}) & F_{22}(\mathbf{l}) \end{vmatrix} \qquad (89)$$

whose components are

$$F_{11}(\mathbf{l}) \equiv G^1(\mathbf{l}) - G^1(\mathbf{l}-\mathbf{i}) = K_0(\mathbf{l}+\mathbf{i}) - 2K_0(\mathbf{l}) + K_0(\mathbf{l}-\mathbf{i}) \quad (90a)$$

$$F_{12}(\mathbf{l}) \equiv G_0{}^1(\mathbf{l}) - G_0{}^1(\mathbf{l}-\mathbf{j})$$
$$= K_0(\mathbf{l}+\mathbf{i}) - K_0(\mathbf{l}) - K_0(\mathbf{l}+\mathbf{i}-\mathbf{j}) + K_0(\mathbf{l}-\mathbf{j}) \quad (90b)$$

$$F_{21}(\mathbf{l}) \equiv G_0{}^2(\mathbf{l}) - G_0{}^2(\mathbf{l}-\mathbf{i})$$
$$= K_0(\mathbf{l}+\mathbf{j}) - K_0(\mathbf{l}) - K_0(\mathbf{l}-\mathbf{i}+\mathbf{j}) + K_0(\mathbf{l}-\mathbf{i}) \quad (90c)$$

$$F_{22}(\mathbf{l}) \equiv G_0{}^2(\mathbf{l}) - G_0{}^2(\mathbf{l}-\mathbf{j}) = K_0(l+\mathbf{j}) - 2K_0(\mathbf{l}) + K_0(l-\mathbf{j}) \quad (90d)$$

When the nonvanishing ϵ's which correspond to unusual bonds are prescribed one will need to find the appropriate G^1 and G^2 to be substituted into (87) in order to give a final closed form to the propagator $K(l, m)$. To this end we obtain from (87) and the definitions (88a) and (88b) two basic equations to be used for determining the G's:

$$G^1(\mathbf{l}) - G_0{}^1(\mathbf{l}) = i\alpha \sum \{\epsilon(\mathbf{l}'+\mathbf{i}, \mathbf{l}')G^1(\mathbf{l}')F_{11}(\mathbf{l}-\mathbf{l}')$$
$$+ \epsilon(\mathbf{l}'+\mathbf{j}, \mathbf{l}')G^2(\mathbf{l}')F_{12}(\mathbf{l}-\mathbf{l}')\} \quad (91a)$$

$$G^2(\mathbf{l}) - G_0{}^2(\mathbf{l}) = i\alpha \sum \{\epsilon(\mathbf{l}'+\mathbf{i}, \mathbf{l}')G^2(\mathbf{l}')F_{12}(\mathbf{l}-\mathbf{l}')$$
$$\epsilon(\mathbf{l}'+\mathbf{j}, \mathbf{l}')G^2(\mathbf{l}')F_{22}(\mathbf{l}-\mathbf{l}')\} \quad (91b)$$

Let us now consider the case of two abnormal bonds, one horizontal and one vertical, so that

$$\epsilon(\mathbf{l}+\mathbf{i}, \mathbf{l}) \equiv \epsilon_1\, \delta_{\mathbf{l},\mathbf{l}_1} \qquad \text{and} \qquad \epsilon(\mathbf{l}+\mathbf{j}, \mathbf{l}) \equiv \epsilon_2\, \delta_{\mathbf{l},\mathbf{l}_2} \quad (92)$$

Then, from (91)

$$G^1(\mathbf{l}_1) = G_0(\mathbf{l}_1) + i\alpha[\epsilon_1 F_{11}(0)G^1(\mathbf{l}_1) + \epsilon_2 F_{12}(\mathbf{l}_1 - \mathbf{l}_2)G^2(\mathbf{l}_2)] \quad (93a)$$

$$G^2(\mathbf{l}_1) = G_0(\mathbf{l}_1) + i\alpha[\epsilon_1 F_{21}(\mathbf{l}_2 - \mathbf{l}_1)G^1(\mathbf{l}_1) + \epsilon_2 F_{22}(0)G^2(\mathbf{l}_2)] \quad (93b)$$

This pair of equations can be solved for $G^1(\mathbf{l}_1)$ and $G^2(\mathbf{l}_2)$. When the resulting expressions are introduced into

$$K(\mathbf{l}) = K_0(\mathbf{l}) + i\alpha\epsilon_1 G^1(\mathbf{l}_1)G_0{}^1(\mathbf{l}-\mathbf{l}_1-\mathbf{i}) + i\alpha\epsilon_2 G^2(\mathbf{l}_2)G_0{}^2(\mathbf{l}-\mathbf{l}_1-\mathbf{j}) \quad (94)$$

[Eq. (87) incorporating (92)], it is found that

$$K(\mathbf{l}, u) = \Delta_2^{-1} \begin{vmatrix} K_0(\mathbf{l}) & G_0{}^1(\mathbf{l}_1) & G_0{}^2(\mathbf{l}_2) \\ \alpha i\epsilon_1 G_0{}^1(\mathbf{l}-\mathbf{l}_1-\mathbf{i}) & \alpha i\epsilon_1 F_{11}(0) - 1 & \alpha i\epsilon_1 F_{21}(\mathbf{l}_2-\mathbf{l}_1) \\ \alpha i\epsilon_2 G_0{}^2(\mathbf{l}-\mathbf{l}_2-\mathbf{j}) & \alpha i\epsilon_2 F_{12}(\mathbf{l}_1-\mathbf{l}_2) & \alpha i\epsilon_2 F_{22}(0) - 1 \end{vmatrix} \quad (95)$$

We have used the vector notation

$$\mathbf{l} \equiv (l, m), \qquad \mathbf{i} \equiv (1, 0), \qquad \mathbf{j} \equiv 0, 1)$$

$$\Delta_2 = \begin{vmatrix} \alpha i\epsilon_1 F_{11}(0) - 1 & \alpha i\epsilon_1 F_{21}(\mathbf{l}_2-\mathbf{l}_1) \\ \alpha i\epsilon_2 F_{12}(\mathbf{l}_1-\mathbf{l}_2) & \alpha i\epsilon_2 F_{22}(0) - 1 \end{vmatrix} \quad (96)$$

Similar equations exist for the wave function of a plane wave scattered by unusual bonds. We start with the basic wave equation

$$\begin{aligned} d\psi/dt - i\alpha\,\Delta^2\psi &= i\alpha\{\epsilon(\mathbf{l}+\mathbf{i},\mathbf{l})[\psi(\mathbf{l}+\mathbf{i}) - \psi(\mathbf{l})] - \epsilon(\mathbf{l}-\mathbf{i},\mathbf{l})[\psi(\mathbf{l}) - \psi(\mathbf{l}-\mathbf{i})] \\ &\quad + \epsilon(\mathbf{l}+\mathbf{j},\mathbf{l})[\psi(\mathbf{l}+\mathbf{j}) - \psi(\mathbf{l})] - \epsilon(\mathbf{l}-\mathbf{j},\mathbf{l})[\psi(\mathbf{l}) - \psi(\mathbf{l}-\mathbf{j})]\} \end{aligned} \tag{97}$$

If we let

$$\psi(\mathbf{l}) = [\exp(-i\omega t)][\exp(i\mathbf{k}\cdot\mathbf{l}) + F(\mathbf{l})] \tag{98}$$

we obtain the following equation for $F(\mathbf{l})$:

$$\begin{aligned} \omega F(\mathbf{l}) + \alpha\,\Delta^2 F(\mathbf{l}) &= -\alpha(\exp i\mathbf{k}\cdot\mathbf{l})\{\epsilon(\mathbf{l}+\mathbf{i},\mathbf{l})(1 - \exp ik_x) - \epsilon(\mathbf{l}-\mathbf{i},\mathbf{l})(1 - \exp - ik_x) \\ &\quad + \epsilon(\mathbf{l}+\mathbf{j},\mathbf{l})(-1 + \exp ik_x) - \epsilon(\mathbf{l}-\mathbf{j},\mathbf{l})(1 - \exp - ik_x)\} \\ &\quad - \alpha\{\epsilon(\mathbf{l}+\mathbf{i},\mathbf{l})[F(\mathbf{l}+\mathbf{i}) - F(\mathbf{l})] - \epsilon(\mathbf{l}-\mathbf{i},\mathbf{l})[F(\mathbf{l}) - F(\mathbf{l}-\mathbf{i})] \\ &\quad + \epsilon(\mathbf{l}+\mathbf{j},\mathbf{l})[F(\mathbf{l}+\mathbf{j}) - F(\mathbf{l})] - \epsilon(\mathbf{l}-\mathbf{j},\mathbf{l})[F(\mathbf{l}) - F(\mathbf{l}-\mathbf{j})]\} \end{aligned} \tag{99}$$

so that if $F_0(\mathbf{l})$ is the Green's function that satisfies

$$\omega F_0(\mathbf{l}) + \alpha\,\Delta^2 F_0(\mathbf{l}) = \delta_{\mathbf{l},0} \tag{100}$$

then

$$\begin{aligned} F(\mathbf{l}) = \sum_{\mathbf{l}'} \{&\epsilon(\mathbf{l}'+\mathbf{i},\mathbf{l}')(\exp i\mathbf{k}\cdot\mathbf{l})(1 - \exp ik_x) \\ &\times [F_0(\mathbf{l}-\mathbf{l}') - F_0(\mathbf{l}-\mathbf{l}'-\mathbf{i})] \\ &+ \epsilon(\mathbf{l}'+\mathbf{j},\mathbf{l}')(\exp i\mathbf{k}\cdot\mathbf{l})(1 - \exp ik_y) \\ &\times [F_0(\mathbf{l}-\mathbf{l}') - F_0(\mathbf{l}-\mathbf{l}'-\mathbf{j})] \\ &+ \epsilon(\mathbf{l}'+\mathbf{i},\mathbf{l}')[F(\mathbf{l}'+\mathbf{i}) - F(\mathbf{l}')][F_0(\mathbf{l}-\mathbf{l}') - F_0(\mathbf{l}-\mathbf{l}'-\mathbf{i})] \\ &+ \epsilon(\mathbf{l}'+\mathbf{j},\mathbf{l}')[F(\mathbf{l}'+\mathbf{j}) - F(\mathbf{l}')][F_0(\mathbf{l}-\mathbf{l}') - F_0(\mathbf{l}-\mathbf{l}'-\mathbf{j})]\} \end{aligned} \tag{101}$$

Now suppose that there are n defective bonds associated with lattice points $\mathbf{l}_1, \mathbf{l}_2, \ldots, \mathbf{l}_n$ in vector directions $\mathbf{j}_1, \mathbf{j}_2, \ldots, \mathbf{j}_n$ and that the ϵ values of the bonds are $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$. Then (101) can be written as

$$\begin{aligned} F(\mathbf{l}) = \alpha &\sum_{\beta=1}^{n} \epsilon_\beta\,(\exp i\mathbf{k}\cdot\mathbf{l}_\beta)(1 - \exp i\mathbf{k}\cdot\mathbf{j}_\beta) \\ &\times [F_0(\mathbf{l}-\mathbf{l}_\beta) - F_0(\mathbf{l}-\mathbf{l}_\beta-\mathbf{j}_\beta)] \\ &- \alpha \sum_{\beta=1}^{n} \epsilon_\beta[F(\mathbf{l}_\beta+\mathbf{j}_\beta) - F(\mathbf{l}_\beta)][F_0(\mathbf{l}-\mathbf{l}_\beta) - F_0(\mathbf{l}-\mathbf{l}_\beta-\mathbf{j}_\beta)] \end{aligned} \tag{102}$$

The vector $\mathbf{j}_\beta$ is equal to $\mathbf{i}$ if the βth defect bond is horizontal and $\mathbf{j}$ if it is vertical. Also $\mathbf{k}\cdot\mathbf{j}_\beta = k_x$ if $\mathbf{j}_\beta \equiv \mathbf{i}$ and k_y if $\mathbf{j}_\beta = \mathbf{j}$.

We also find that

$$\begin{aligned} F(\boldsymbol{l}_\gamma + \mathbf{j}_\gamma) - F(\boldsymbol{l}_\gamma) &= \alpha \sum_\beta \epsilon_\beta (\exp i\mathbf{k}\cdot\boldsymbol{l}_\beta)(1 - \exp i\mathbf{k}\cdot\mathbf{j}_\beta) U_{j_\gamma j_\beta}(\boldsymbol{l}_{\gamma\beta}) \\ &\quad + \alpha \sum_\beta \epsilon_\beta [F(\boldsymbol{l}_\beta + \mathbf{j}_\beta) - F(\boldsymbol{l}_\beta)] U_{j_\gamma j_\beta}(l_{\gamma\beta}) \end{aligned} \tag{103}$$

where $\boldsymbol{l}_{\gamma\beta} = \boldsymbol{l}_\gamma - \boldsymbol{l}_\beta$ and

$$U_{jk}(\boldsymbol{l}) \equiv F_0(\boldsymbol{l} + \mathbf{j}) - F_0(\boldsymbol{l} - \mathbf{j} + \mathbf{k}) - F_0(\boldsymbol{l}) + F_0(\boldsymbol{l} - \mathbf{k}) \tag{104}$$

Since the Green's functions $F_0(\boldsymbol{l})$ are postulated to be known, the function $F(\boldsymbol{l})$ will also be known if the values of

$$F(\boldsymbol{l}_\beta + \mathbf{j}_\beta) - F(\boldsymbol{l}_\beta) \equiv H_\beta \tag{105}$$

can be determined in terms of the $F_0(\boldsymbol{l})$. This can be accomplished by noting that (103) is a set of linear equations for just these variables. If we define

$$W_\gamma(\boldsymbol{l}_\gamma) \equiv \alpha \sum_\beta \epsilon_\beta (\exp i\mathbf{k}\cdot\boldsymbol{j}_\beta)(1 - \exp i\mathbf{k}\cdot\mathbf{j}_\beta) U_{j_\gamma j_\beta}(l_{\gamma\beta}) \tag{106}$$

then (103) bcomes

$$W_\gamma(\boldsymbol{l}_\gamma) = \sum_{\beta=1}^{n} k_{\gamma\beta} H_\beta \tag{107}$$

where we have set (with $\gamma, \beta = 1, 2, \ldots, n$)

$$k_{\gamma\beta} \equiv \alpha\epsilon_\beta U_{j_\gamma, j_\beta}(\boldsymbol{l}_{\gamma\beta}) + \delta_{\gamma\beta} \tag{108}$$

Then

$$H_1 = \begin{vmatrix} W_1(\boldsymbol{l}_1) & k_{12} & \cdots & k_{1n} \\ W_2(\boldsymbol{l}_2) & k_{22} & \cdots & k_{2n} \\ \vdots & & & \\ W_n(\boldsymbol{l}_n) & k_{n2} & \cdots & k_{nn} \end{vmatrix} \begin{vmatrix} k_{11} & k_{12} & \cdots & k_{1n} \\ k_{21} & k_{22} & \cdots & k_{2n} \\ \vdots & & & \\ k_{n1} & k_{n2} & \cdots & k_{nn} \end{vmatrix} \tag{109}$$

etc. When these expressions are substituted into (102) it is found that

$$F(\boldsymbol{l}) = D_n/\Delta_n \tag{110}$$

where

$$D_n \equiv \begin{vmatrix} k_{00} & k_{10} & \cdots & k_{n0} \\ k_{01} & k_{11} & \cdots & k_{n1} \\ \vdots & & & \\ k_{0n} & k_{1n} & \cdots & k_{nn} \end{vmatrix}; \qquad \Delta_n \equiv \begin{vmatrix} k_{11} & k_{21} & \cdots & k_{n1} \\ k_{12} & k_{22} & \cdots & k_{n2} \\ \vdots & & & \\ k_{1n} & k_{2n} & \cdots & k_{nn} \end{vmatrix} \tag{111}$$

with $k_{\gamma\beta}$ being defined by (108) when $\gamma, \beta = 1, 2, \ldots, n$, and with $j = 1, 2, \ldots, n$,

$$k_{j0} \equiv W_j(\boldsymbol{l}_j) \qquad \text{and} \qquad k_{0\beta} \equiv \alpha\epsilon_\beta H(\boldsymbol{l}, \beta) \tag{112}$$

where

$$H(\mathbf{l}, \beta) \equiv [F(\mathbf{l} - \mathbf{l}_\beta) - F(\mathbf{l} - \mathbf{l}_\beta - \mathbf{j}_\beta)]$$

$$k_{00} \equiv \alpha \sum_{\beta=1}^{n} \epsilon_\beta(\exp i\mathbf{k}\cdot\mathbf{l}_\beta)(1 - \exp i\mathbf{k}\cdot\mathbf{j}_\beta) \times [F_0(\mathbf{l} - \mathbf{l}_\beta) - F(\mathbf{l} - \mathbf{l}_\beta - \mathbf{j}_\beta)]$$

While the derivation of (110) was for a two-dimensional lattice the result is also correct for a three-dimensional one. In that case, the unit vectors $\mathbf{j}_\beta$ may be $\mathbf{i}$, $\mathbf{j}$, or $\mathbf{k}$, depending on the direction of the βth unusual bond. The vector $\mathbf{l}$ has three components $\mathbf{l} \equiv (l_1, l_2, l_3)$. Also $\mathbf{k}\cdot\mathbf{j}_\beta = k_x$ if $\mathbf{j}_\beta = \mathbf{i}$, k_y if $\mathbf{j}_\beta = \mathbf{j}$, and k_z if $\mathbf{j}_\beta = \mathbf{k}$. The Green's function $F_0(\mathbf{l})$ defined by (100) is a three-dimensional one and the Δ^2 is to be interpreted as the three-dimensional Laplace difference operator.

We have thus reduced the calculation of the scattered component of the wave function $F(\mathbf{l})$ to quadratures. However, detailed numerical work requires formulas for the Green's function $F_0(l)$. We now proceed to develop some of these.

5. REMARKS ON THE LATTICE GREEN'S FUNCTION

The wave function of a wave scattered by unusual regions (bonds or points) in a periodic lattice space through which waves may propagate has been expressed as a ratio of two determinants. If the individual determinants in (109) are expanded in powers of an ϵ which measures the deviation of the bond parameters of unusual bonds from normal ones, the resulting expression for the scattered wave functions is a ratio of two polynomials in ϵ, a form which is often postulated when the method of Padé approximants is used.

While our formula for the scattered wave function has been reduced to quadratures, actual numerical calculations using the formula require expressions for the lattice Green's functions. Such Green's functions have been vigorously studied in recent years since they occupy a basic position in solid state theory. In this section we collect a number of relevant properties of the Green's functions $F_0(\mathbf{l}, \omega)$ and $K_0(\mathbf{l}, u)$ defined by (100), (45), (36), and (55).

The scattered wave Green's function, $(\exp -i\omega t)F_0(\mathbf{l}, \omega)$, defined so that in one dimension $F_0(\mathbf{l})$ satisfies (45) and in three dimensions satisfies (100),

$$\omega F_0(\mathbf{l}, \omega) + \alpha\,\Delta^2 F_0(\mathbf{l}, \omega) = \delta_{\mathbf{l},0} \tag{113}$$

must, at points l far from the origin, have the form of outgoing waves receding in all directions from the origin. Hence, one should have

$$(\exp -i\omega t)F_0(l, \omega) \sim \begin{cases} g_1(k)\exp[-i(\omega t - k|l|) & \text{1D} \\ g_3(\mathbf{k})|\mathbf{l}|^{-1}\exp[-i(\omega t - k|\mathbf{l}|)] & \text{3D} \end{cases} \tag{114}$$

where $g_1(k)$ and $g_3(\mathbf{k})$ are functions which might depend on **k** but which for large $|\boldsymbol{l}|$ must be independent of $|\boldsymbol{l}|$.

The function

$$F_0(l) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\exp(il\phi)\, d\phi}{\omega + i\epsilon - 2\alpha(1 - \cos\phi)} \tag{115}$$

as $\epsilon \to 0$ satisfies (45) if

$$\omega = 2\alpha(1 - \cos k) \tag{116}$$

Since

$$F_0(l) = F_0(-l) \tag{117}$$

we need only consider the case $l \geqslant 0$. We now show that the form (115) when multiplied by $\exp(-i\omega t)$ represents an outgoing wave. Let $z_0 = \exp i\phi$. Then (C being a counterclockwise unit circle contour)

$$F_0(l) = \frac{1}{2\pi i\alpha}\int_C \frac{z^l dz}{z^2 - z(z_0 + z_0^{-1} - 2i\epsilon) + 1} \tag{118}$$

The poles of the integrand, when $l \geqslant 0$, are at

$$z_\pm = z_0^{\pm 1}\{1 \mp (\epsilon/\sin k) + O(\epsilon^2)\} \tag{119}$$

Hence z_+ lies inside the contour if $0 < k < \pi$ and z_- lies outsize. Then from the theory of residues

$$F_0(l) = e^{ikl}/(2i\alpha \sin k) \qquad \text{if} \quad l > 0 \tag{120a}$$

From (117)

$$F_0(l) = e^{ik|l|}/(2i\alpha \sin k) \qquad \text{for all real integral } l \tag{120b}$$

which is consistent with (114) if $g_1(k) = (2i\alpha \sin k)^{-1}$.

We now show, as $\epsilon \to 0$ (with $c_j \equiv \cos l_j$) that the function

$$F_0(\boldsymbol{l}) = \frac{1}{(2\pi)^3}\iiint_{-\pi}^{\pi} \frac{\exp(i\boldsymbol{l}\cdot\boldsymbol{\phi})\, d^3\boldsymbol{\phi}}{\omega + i\epsilon - 2\alpha(3 - c_1 - c_2 - c_3)} \tag{121}$$

which satisfies (113) and has the required form (114). Note also that since[2,16]

$$x^{-1} = \int_0^\infty \exp - xz\, dz \tag{122}$$

then

$$F_0(\boldsymbol{l}) = \frac{1}{i(2\pi)^3}\int_0^\infty \exp[-z(\epsilon - i\omega)]\, dz$$
$$\times \prod_{j=1}^{3}\int_{-\pi}^{\pi} \exp\{i[l_j\phi_j - 2\alpha z(1 - c_j)]\}\, dl_j \tag{123}$$

This function can be reduced to a single integral by using the integral representation of the Bessel function

$$2\pi i^l J_l(y) = \int_{-\pi}^{\pi} e^{iy\cos l} \cos l\phi \, d\phi \tag{124}$$

One then obtains

$$F_0(\mathbf{l}) = i^{l_1+l_2+l_3-1} \int_0^\infty J_{l_1}(2\alpha z) J_{l_2}(2\alpha z) J_{l_3}(2\alpha z) e^{-z(\epsilon - i[\omega - 6\alpha])} \, dz \tag{125}$$

When the l_j are very large there is some merit in introducing a lattice spacing into our model by writing $\alpha = \lambda/a^2$, for then in the limit $a \to 0$, Eq. (21) becomes the Schrödinger equation. When the l_j are large the integrands of the ϕ integrals of (123) oscillate rapidly except when $|\boldsymbol{\phi}|$ is very small. Hence we can use the approximation

$$\exp[-2\alpha z i(1 - c)] \sim \exp[-i\alpha z(\phi^2 - \tfrac{1}{12}\phi^4 + \cdots)] \tag{126}$$

Then a typical one of our required integrals in (123) becomes

$$\int_{-\pi}^{\pi} \exp\{-i[z\lambda(\phi/a)^2 - la(\phi/a) - za^2(\phi/a)^4 + \cdots]\} \, d\phi \tag{127}$$

Now we introduce a fixed length r with

$$\mathbf{r} = a\mathbf{l} \qquad \text{and set} \quad (\phi/a) \equiv x \tag{128}$$

If a is made small and $\mathbf{l}$ large, keeping $\mathbf{r}$ fixed, then (127) becomes

$$a\int_{-\pi/a}^{\pi/a} \exp[-i(z\lambda x^2 - rx - za^2x^4 + \cdots)] \, dx \tag{129}$$

Hence as a becomes very small the limits of integration can be made $(-\infty, \infty)$ and all terms of order x^4 and greater can be neglected in the integrand. On this basis, with

$$\mathbf{r}^2 \equiv a^2(l_1{}^2 + l_2{}^2 + l_3{}^2) \equiv a^2\mathbf{l}^2 \tag{130}$$

Eq. (127) becomes

$$\int_{-\infty}^{\infty} \exp[-i(z\lambda x^2 - rx)] \, dx = a(\pi/\lambda z)^{1/2} \exp(-\tfrac{1}{4}i\pi + ir^2/\lambda z) \tag{131}$$

Then, if we rewrite $\alpha = \lambda/a^2$, (123) becomes

$$\begin{aligned} F_0(l) &\sim [\exp(-\tfrac{3}{4}i\pi)/8i(\pi\alpha)^{3/2}] \\ &\quad \times \int_0^\infty z^{-3/2} \exp\{i[z(\omega + i\epsilon) + (r^2/\lambda z)]\} \, dz \\ &= (8\pi l\alpha)^{-1} \exp[2il(\omega/\alpha)^{1/2}] \end{aligned} \tag{132}$$

which is of the required form (114).

Rays that propagate from the scattering region to a distant point of observation correspond to large $\boldsymbol{l}$, for which (132) is valid. Rays that represent internal scattering between unusual bonds would correspond to small $\boldsymbol{l}$ values. The function $F_0(0)$ which is found in scattering formulas such as (69) and (110) was first tabulated by Koster and Slater.[2] A more extensive table has been prepared by Joyce.[15] The symmetries of our problem tell us that

$$F_0(0, 0, \pm 1) = F_0(0, \pm 1, 0) = F_0(\pm 1, 0, 0) \tag{133}$$

These functions can in turn be found from $F_0(0, 0, 0)$ by using the recurrence formula

$$F_0(1, 0, 0) = [1 - (\omega - 6\alpha)F_0(0, 0, 0)]/6\alpha \tag{134}$$

The general recurrence formula (113) is useful for calculating $F_0(\boldsymbol{l})$ from diagonal F_0's such as $F_0(s, s, s)$.

Certain series expansions for products of Bessel functions expedite[10] the derivation of formulas for $F_0(\boldsymbol{l})$ for $\boldsymbol{l}$ values too small for the application of (132). For example, the series

$$J_\mu(z)J_\nu(z) = \sum_{k=0}^{\infty} \frac{(-1)^k(\mu + \nu + 2k)!\,(\tfrac{1}{2}z)^{\mu+\nu+2k}}{(\mu + \nu + k)!\,(\nu + k)!\,(\mu + k)!\,k!} \tag{135}$$

yields

$$F_0(l) = i^{l_1+l_2+l_3-1} \sum_{k=0}^{\infty} \int_0^\infty \frac{(-1)^k(l_1 + l_2 + 2k)!\,(\alpha z)^{l_1+l_2+2k} J_{l_3}(2\alpha z)e^{-\gamma z}\,dz}{(l_1 + l_2 + k)!\,(l_1 + k)!\,(l_2 + k)!\,k!} \tag{136}$$

with

$$\gamma = \epsilon - i(\omega - 6\alpha) \tag{136a}$$

Since

$$\int_6^\infty e^{-\gamma x}J_\gamma(\beta x)x^{s-1}\,dx = (\gamma^2 + \beta^2)^{-s/2}\Gamma(\lambda + s)P_{s-1}^{-\lambda}[\gamma(\gamma^2 + \beta^2)^{-1/2}]$$

then

$$F_0(l) = i^{l_1+l_2+l_3-1} \times \sum_{k=0}^{\infty} \frac{(-1)^k(l_1+l_2+2k)!(l_1+l_2+l_3+2k)!\,\alpha^{l_1+l_2+2k}P^{-l_3}_{l_1+l_2+2k}(v)}{k!(l_1+l_2+k)!(l_1+k)!(l_2+k)![4a^2-(\omega-6\alpha)^2]^{1/2}(l_1+l_2+2k+1)} \tag{137}$$

with

$$v \equiv \gamma/(\gamma^2 + \beta^2)^{1/2} = [(6\alpha - \omega)^2/(8\alpha - \omega)(4\alpha - \omega)]^{1/2}$$

and $P_{s-1}^{-\lambda}(v)$ is an associated Legendre function of the first kind. Other expansion forms are also available for the computation of $F_0(l)$. The bases of these are discussed in Ref. 10.

When the Green's functions needed for the calculation of the scattered wave function involve a number of vectors (l_1, l_2, l_3) it seems to be most efficient to use (137) or an alternative formula to calculate the minimum set $F_0(l, l, l)$ required to obtain, using the recurrence formula (113), the $F_0(l_1, l_2, l_3)$ for the required vectors.

6. CONCLUSIONS

We have investigated the theory of propagation of waves in a periodic lattice space which contains limited regions of traps or unusual bonds between lattice points. Generally the scattered wave function is a ratio of determinants with the number of rows and columns being of the order of the number of unusual points or bonds. The elements of the determinants are related to lattice Green's functions for which formulas and tables exist. The detailed application of the formulas to a number of special scattering problems will be given in related publications.

Let us now consider the connection between our expression for the scattered wave function as a ratio of determinants and various other formulations of scattering theory.

First imagine taking the limit as the number of defective lattice bonds in the interior of the scattering region approaches infinity while the lattice spacing a approaches zero. This corresponds to proceeding to the continuum limit of our model. In that case the original scattering process would have been described by an integral equation and our ratio of determinants (which now become infinite determinants) would be equivalent to the Fredholm determinant solution of the scattering integral equation. While this form of scattering theory was discussed by Jost and Pais[17] many years ago, it is seldom applied to specific problems.

If the ratio of the determinants (110) is expanded in powers of ϵ_j and all terms of second or higher order are neglected, the result corresponds to the Born approximation.

When many wavelengths of the incident wave fit into the range of the scatterer the determinants in (110) become large so that our method is not particularly efficient. However, if the ϵ_j are small while the range of the potential is large, the eikonal approximation is suitable for the discussion of the scattering problem. In another publication we will introduce exponential generating functions for determinants and from them derive the discrete analog of the eikonal approximation. This will represent a certain approximation to large determinants.

Discrete analogs of Maxwell's equations, the Dirac equation, and the wave equation for sound propagation can be derived. These will be used in other reports to investigate the scattering of light, electrons, and sound by certain models of scattering centers as well as by surfaces.

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