Isolated defects in the static limit

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Abstract. We collect together the known results for the effect of a single defect into a single
compact form that can be used in any lattice in the static limit. The result is used to calculate
the effect of single defects (either bonds or sites) on the diffusion constant and conductivity
of various lattices. It is shown that the result of Izyumov for the spin-wave stiffness can be
simply generalised to any lattice.

1. Introduction

The effect of a single impurity on some desired response function is well understood
(see, for example, Elliott et al 1974). Practical calculations are possible if the range over
which the interactions are changed by the impurity is very short. In general, the detailed
symmetry around the defect site must be taken into account in order to complete the
calculation. An exception is a mass defect, where a simple formula can be written down
that is valid for any lattice. The lattice only comes in when the particular on-site Green
function needed is calculated. Another similar situation is provided by a site diagonal
impurity in a tight-binding model (see, for example, Economu 1979).

In this paper, we look at two other cases that can also be carried through without
worrying about the particular lattice until the pure lattice Green function has to be
evaluated.

The first of these is the bond defect in a tight-binding model, a result given by
Kirkpatrick (1973). A more interesting and complex example is a site defect when a site
and all its bonds to its nearest neighbours are altered.

2. General formalism

For convenience, we consider a system described by a vibrational potential

$$U = \sum_{i\alpha\beta} A_{\alpha\beta}^i u_i^\alpha u_i^\beta$$

(1)

where all the atoms are mass points with mass $m$; $i$ and $j$ are sites, and $\alpha$ and $\beta$ are
Cartesian components. The vector $u_i$ is the displacement on the $i$th site. The $A_{\alpha\beta}^i$ are
subject to various symmetry restrictions that we do not need to consider here. We shall
switch to tight-binding language later. The dynamical matrix for this system is defined from the equation of motion

\[ m\omega^2 u_\omega = \sum_{\beta} A_{\omega \beta} u_\beta \]  

(2)

or

\[ m\omega^2 u = Du \]  

(2a)

where \( u \) is considered to be a \( dN \)-dimensional vector. The dimensionality of the system is \( d \) and there are \( N \) atoms. The \( dN \times dN \) matrix \( D \) is the usual dynamical matrix (see, for example, Born and Huang 1966).

If a force \( f_e \), also considered as a \( dN \) vector, is externally applied to the system, then

\[ f_e = -f = Du. \]  

(3)

We shall be considering only cases where \( f_e \) (and hence \( f \) the force produced by the system to oppose \( f_e \) in equilibrium) is non-zero at the surface. Inverting equation (3), we find that

\[ u = Gf \]  

(4)

where \( G \) is the zero-frequency limit of the usual Green function \( G(\omega^2) \) given by

\[ G(\omega^2) = (m\omega^2 - D)^{-1}. \]  

(5)

As we are only concerned with the static limit, the masses are irrelevant and so we shall set them all equal to \( m \). If the system described by (1) consists of a perfect crystal with a dynamical matrix \( D_0 \) plus a defect, where the defect has a (localised) potential \( V \), then we have the usual Dyson equation

\[ G = P + PVG \]  

(6)

where \( D = D_0 + V \). Here \( P \) is the perfect crystal Green function and \( G \) is the Green function of the system plus defect. Note that \( D_0 P = DG = -I \). We may solve (6) formally:

\[ G = (1 - PV)^{-1} P. \]  

(7)

The static energy \( E' \) of the system produced by the application of the external force \( f_e \) is

\[ E' = \frac{1}{2} f_e \cdot u = -\frac{1}{2} f \cdot Gf. \]  

(8)

We see from (6) and (7) that

\[ G - P = PVG = PV(1 - PV)^{-1} P. \]

The change \( \Delta E = E' - E \) in the energy due to the presence of the defect is therefore

\[ \Delta E = -\frac{1}{2} f \cdot (G - P)f = -\frac{1}{2} f \cdot PV(1 - PV)^{-1} Pf. \]  

(9)

This form is quite convenient as usually \( f \) is only non-zero at the surface of the sample. However, a better form for our purposes is obtained by writing the equation similar to (4) but for the perfect system

\[ u_0 = Pf \]  

(10)

where \( u_0 \) are the displacements produced by the force \( f \) before the defect was introduced and using this we can write

\[ \Delta E = -\frac{1}{2} u_0 \cdot V(1 - PV)^{-1} u_0. \]  

(9a)
This result can be rewritten using the $T$ matrix:

$$T = V(1 - PV)^{-1}$$  \hspace{1cm} (11)

as

$$\Delta E = -\frac{1}{2} u_0 \cdot T \cdot u_0.$$  \hspace{1cm} (12)

This is a very convenient form for developing effective medium theories of many defects as well as the single-defect problem that we are considering here. Equation (12) is simple because the range of $T$ is the same as that of $V$ and so is localised around the defect. In order to calculate $\Delta E$, it is therefore only necessary to know $u_0$ around the defect. Remember that the $u_0$ are the displacements produced by the external force $f_e$ in the absence of the defect. When the defect is introduced, the force $f$ is held constant and the strain changes. The situation is particularly simple in a Bravais lattice if $f_e$ is a uniform external stress (e.g. shear or compression). Then the lattice distortion is homogeneous and $u_0$ is very easy to write down. This is the only case that we shall be considering here.

3. Isotropic Born model

We apply the work of § 2 to the isotropic Born (1914) model, where the perfect lattice is described by the potential

$$U = \frac{\alpha}{4} \sum_{i,j} (u_i - u_j)^2$$  \hspace{1cm} (13)

and the sum is restricted to nearest neighbours. This model decouples in the $d$ orthogonal Cartesian directions into $d$ separate tight-binding Hamiltonians:

$$H = \frac{\alpha}{2} \sum_{i,j} (a_i^+ a_i - a_i^+ a_j)$$  \hspace{1cm} (14)

where the sums in (13) and (14) go over $j$ which are nearest neighbours of $i$, which is also summed over. We shall work in the language of the isotropic Born model and 'translate' into tight-binding language later. This is convenient as stresses and homogeneous strains are easier to visualise than the equivalent in the tight-binding model.

Let us consider a uniform strain $u_0$ in which the $i$th atom has a displacement

$$u_i = \varepsilon R_i$$  \hspace{1cm} (15)

where $\varepsilon$ is the magnitude of the strain. This homogeneous strain (15) is appropriate for any Bravais lattice. Because all homogeneous strains (i.e. shear, compression, etc) for the potential (13) are trivially related, we use the simple form (15) where $\varepsilon$ is a scalar. The methods outlined here become a little more complex for lattices with a basis where the strain is not usually homogeneous. Inserting (15) into (13), we find that the strain energy $E$ is given by

$$E = \frac{1}{4} \alpha \varepsilon^2 N z a^2$$  \hspace{1cm} (16)

where $a$ is the separation of the $z$ nearest neighbours. Note that the origin used for the external strain (15) is irrelevant as only differences in displacements contribute towards the strain energy (16).
4. Bond defect

We now consider a very simple defect. A single bond is changed from \( \alpha \rightarrow \alpha_0 \). We shall number the atoms 1 and 2 as in figure 1. In general the strain (15) will produce

\[
\begin{align*}
\vec{u}_1 & = -\vec{u}_2 = \frac{1}{2} \varepsilon \mathbf{R}_{12} \\
\mathbf{R}_{12} & = \mathbf{R}_1 - \mathbf{R}_2
\end{align*}
\]

Figure 1. The two displacements \( \vec{u}_1 \) and \( \vec{u}_2 \) produced by a uniform external stress around a single altered bond. These are the components of the vector \( |s\rangle \).

Because the defect is localised, no other displacements need to be used as basis functions in (9a). It is convenient to choose the centre of the bond 1–2 as the origin for the strain. This excludes any uniform motion of the defect bond, which may be included, but does not contribute to (9a). On this basis (Feng et al 1985), the \( \mathbf{V} \) matrix may be written

\[
\mathbf{V} = (\alpha_0 - \alpha) \begin{pmatrix}
1 & -1 \\
-1 & 1
\end{pmatrix}
\]

and

\[
\begin{align*}
\vec{u}_0 & = \varepsilon a \begin{pmatrix}
\frac{1}{2} \\
-\frac{1}{2}
\end{pmatrix} \\
\vec{u}_0 & = (\varepsilon a/2^{1/2}) |s\rangle
\end{align*}
\]

where

\[
|s\rangle = \begin{pmatrix}
1 \\
2^{1/2} \\
-1 \\
2^{1/2}
\end{pmatrix}
\]

so that the state vector \( |s\rangle \) is properly normalised. Note that

\[
\mathbf{V}|s\rangle = 2(\alpha_0 - \alpha)|s\rangle
\]

so that

\[
\Delta E = -\frac{1}{4} \varepsilon^2 a^2 \{ 2(\alpha_0 - \alpha) / [1 - 2(\alpha_0 - \alpha)|s\rangle \langle s| P |s\rangle] \}
\]

where we have also used the fact that \( |s\rangle \) is an eigenvector of \( P \). This happens because the two states on the atoms 1 and 2 transform as a symmetric and an antisymmetric vector under the symmetry group of the bond. Because there is a single representation of each kind, there is no mixing so that the antisymmetric vector \( |s\rangle \) must be the eigenstate of \( P \). The symmetric representation corresponds to the uniform translation and so is irrelevant. This type of argument becomes much more powerful in the site defect case to be considered later.
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Therefore,
\[
\langle s | P | s \rangle = \frac{1}{4} (P_{11} + P_{22} - P_{12} - P_{21})
\]
\[
= P_{11} - P_{12}
\]
by symmetry, where
\[
P_{\mathbf{q}} = \frac{1}{N} \sum_{\mathbf{k}} \frac{\exp(i\mathbf{k} \cdot \mathbf{R}_\mathbf{q})}{m(\omega^2 - \omega_k^2)}
\]
(23)
and
\[
m\omega_k^2 = \alpha z(1 - \gamma_k)
\]
(24)
where
\[
\gamma_k = \frac{1}{z} \sum_{\mathbf{\delta}} \exp(i\mathbf{k} \cdot \mathbf{\delta})
\]
(25)
and \(\mathbf{\delta}\) are the \(z\) nearest-neighbour vectors. The excitations (24) are just those of the pure isotropic Born model. In general the \(P_{\mathbf{q}}\) must be evaluated numerically, but in the present case we can make a short-cut by using the equation of motion for \(P_{11}\):
\[
m\omega^2 P_{11} = 1 + z\alpha (P_{11} - P_{12})
\]
(26)
so that, as \(\omega^2 \to 0\), \(P_{11} - P_{12} = - (z\alpha)^{-1}\) and hence
\[
\Delta E = - \frac{1}{4} e^2 a^2 [(\alpha_0 - \alpha)/[1 + 2(\alpha_0 - \alpha)/z\alpha]].
\]
(27)

If we remember that, when the defect is introduced, the stress is held constant, it is the quantity \(1/\alpha\) that is renormalised as the energy is proportional to \(f^2/\alpha\). Hence, we may write
\[
\alpha/\alpha_c = E'/E = 1 + \Delta E/E = 1 + f \cdot \mathbf{P} \cdot \mathbf{T} \cdot \mathbf{f} / f \cdot \mathbf{P} \cdot \mathbf{f}
\]
(28)
using equations (9) and (11). This can be written in terms of the \(u_0\) produced by the \(f\):
\[
\frac{\alpha}{\alpha_c} = 1 - u_0 \cdot \mathbf{T} \cdot u_0 / u_0 \cdot \mathbf{D} \cdot u_0.
\]
(29)

This result is quite general. We find that in the present case
\[
\frac{\alpha}{\alpha_c} = 1 - \frac{1}{4} N_0 e^2 a^2 [(\alpha_0 - \alpha)/[1 + 2(\alpha_0 - \alpha)/z\alpha]]
\]
\[
= 1 - c(\alpha_0 - \alpha)/[\alpha + 2(\alpha_0 - \alpha)/z]
\]
(30)
where \(N_0 = \frac{1}{2} Ncz\) is the (small) number of non-interacting defects. It is more usual to invert (30) to give
\[
\alpha_c = \alpha + c(\alpha_0 - \alpha)/[1 - 2(\alpha_0 - \alpha)(s|P|s)]
\]
\[
= \alpha + c(\alpha_0 - \alpha)/[\alpha + 2(\alpha_0 - \alpha)/z]
\]
(30a)
to first order in the concentration \(c\) of defects. This has been obtained previously by Kirkpatrick (1973) but serves to illustrate the method.

A particularly interesting case occurs for a missing bond \((\alpha_0 = 0)\) when
\[
\alpha_c = \alpha - ca/(1 - 2/z)
\]
(31)
which extrapolates to zero at
\[ c_1 = 1 - \frac{2}{z} \]
or
\[ p_1 = 1 - c_1 = \frac{2}{z}. \] (32)

This is the intercept in a plot of \( \alpha \) against \( p \) when the initial slope is extrapolated to where it crosses the horizontal axis. This is discussed in more detail in § 4. If we go back to (21), an alternative expression for \( p_1 \) is given by
\[ p_1 = -2\alpha(s)P|s| \] (32a)

where \( |s| \) is the state vector characterising the local strain around the defect but in the absence of the defect, and \( P \) is the perfect crystal Green function. This form is useful as a similar but distinct form holds for a site vacancy. The place where \( \alpha_c \) actually goes to zero is of course the percolation concentration \( p_c \). Kirkpatrick (1973) has shown that the conductance of a network of wires behaves as \( \alpha_c \) if we identify the tight-binding parameter (or in our case the spring constant) \( \alpha \) with the conductance of a wire joining adjacent sites. Kirkpatrick has also shown that the diffusion constant \( D \) can be obtained from \( G \) via
\[ G = P_s D \] (33)

where \( P_s \) is the probability that a site is connected into the infinite cluster. Throughout this paper, we shall use units such that \( G \) and \( D \) are normalised to unity at \( p = 1 \). This saves having to write \( G/G_0 \) and \( D/D_0 \) everywhere. It is easy to calculate \( P_s \) for small \( c \) in the present case. To isolate a site, it must have all \( z \) bonds cut; therefore
\[ P_s = 1 - c^z + O(c^{2z-1}) \] (34)

and so makes no contribution to \( O(c) \). Therefore the initial slope of the diffusion constant \( D \) is the same as that of the conductance \( G \) and the extrapolated intercept \( p'_1 \) is just given by
\[ p'_1 = p_1. \] (35)

In table 1, we give \( p_c, p_1 \) and \( p'_1 \) for some common Bravais lattices. The quantities \( G, D \) and \( P_s \) all go to zero at \( p_c \). If \( G \sim (p - p_c)^c, D \sim (p - p_c)^c \) and \( P_s \sim (p - p_c)^c \), then

<table>
<thead>
<tr>
<th>Lattice</th>
<th>( p_c )</th>
<th>( p_1 )</th>
<th>( p'_1 )</th>
<th>( p_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear chain</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Square net</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Triangular net</td>
<td>0.347</td>
<td>0.333</td>
<td>0.333</td>
<td>0.333</td>
</tr>
<tr>
<td>SC</td>
<td>0.247</td>
<td>0.333</td>
<td>0.333</td>
<td>0.333</td>
</tr>
<tr>
<td>BCC</td>
<td>0.179</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>FCC</td>
<td>0.119</td>
<td>0.167</td>
<td>0.167</td>
<td>0.167</td>
</tr>
<tr>
<td>( d = 4 ) hypercube</td>
<td>0.160</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>( d = \infty ) hypercube</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1. The percolation concentration \( p_c \), the intercept \( p_1 \) of the extrapolated initial slope for the conductance \( G \), the intercept \( p'_1 \) of the extrapolated initial slope for the diffusion constant \( D \) and the intercept \( p_1 \) of the extrapolated initial slope in the superconducting limit.

It will be helpful to glance at figures 3 and 4 to see what these are. All values are for bond percolation. The values of \( p_c \) are from Zallen (1983).
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t' = t - \beta. In 2D, t = 1.3 and \beta = 0.14 whereas, in 3D, t = 1.9 and \beta = 0.4 from Stauffer (1985, and references therein). These indices depend only on dimensionality and are the same for both site and bond percolation.

Finally, in this section, we note that the relation \( G = \rho v^2_s \) is the analogue of

\[ E = \rho v^2_s \]

where \( E \) is an elastic modulus, \( \rho \) is the mass density and \( v_s \) is the velocity of sound. It is clear that such a mapping exists because of the equivalence of the tight-binding model and the isotropic Born model.

4. Site defect

Using the general ideas in § 3, we can obtain an expression for a general site defect. It is convenient to use a uniaxial rather than a hydrostatic strain as in § 3, so that the \( i \)th atom has a displacement

\[ u_i = \varepsilon(R_i \cdot \hat{x}) \hat{y} \]

where \( \hat{x} \) and \( \hat{y} \) are any directions; these need not be orthogonal and they can be the same. Also, \( \hat{y} \) may be perpendicular to the lattice (e.g. the z direction for a 2D network in the \( (x, y) \) plane). In that case the isotropic Born potential (13) must also contain terms in the \( z \) direction. All this arbitrariness is because of the isotropy which leads to a single diffusion constant or elastic stiffness. This formalism can also be used with anisotropic interactions, such as central forces, in which case careful track must be kept of directions (Thorpe and Garboczi 1987).

The strain energy of the system, using (13) and (37), is

\[ E = \frac{1}{2} \varepsilon^2 Nz a^2 / d. \]

The vector \( u_b \) is formed from the homogeneous strain (37). All the \( z \) bonds around the defect site have force constants \( a_b \), while all the other bonds have the original force constants \( a \). It is convenient to choose the origin at the centre of the defect (figure 2). As in the bond case, this does not affect the result but simplifies the algebra. The nearest neighbours of the central site have displacements

\[ u_b = \varepsilon(R \cdot \hat{x}) \hat{y} \]

![Diagram](image.png)

**Figure 2.** The displacements produced by a uniform uniaxial external stress in a triangular lattice around a single altered site. These are the components of the vector \( \delta \).
where \( \delta \) goes over the \( z \) nearest-neighbour vectors each of length \( a \). The normalisation is given by

\[
\sum_\delta \mathbf{u}_\delta^3 = \varepsilon^2 \sum_\delta (\delta \cdot \mathbf{x})^2 = \varepsilon z a^2 / d
\]  

(40)

if all \( d \) directions are equivalent. This is true for all the cases to be considered here and listed in table 2. Thus we are restricted to Bravais lattices in which a second-rank tensor is a constant multiplied by the unit matrix. The formalism becomes a little more complex in other situations but can still be used. We may write the state vector \(|s\rangle\) as

\[
\mathbf{u}_0 = \varepsilon a (\mathbf{x}/d^{1/2}) |s\rangle
\]  

(41)

<table>
<thead>
<tr>
<th>Lattice</th>
<th>( p_{cc} )</th>
<th>( p_{t} )</th>
<th>( p_{1}^{t} )</th>
<th>( p_{1}^{c} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear chain</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>Square net</td>
<td>0.593</td>
<td>0.682</td>
<td>0.534</td>
<td>0.182</td>
</tr>
<tr>
<td>Triangular net</td>
<td>0.5</td>
<td>0.641</td>
<td>0.440</td>
<td>0.141</td>
</tr>
<tr>
<td>sc</td>
<td>0.311</td>
<td>0.605</td>
<td>0.347</td>
<td>0.105</td>
</tr>
<tr>
<td>bcc</td>
<td>0.245</td>
<td>0.579</td>
<td>0.273</td>
<td>0.079</td>
</tr>
<tr>
<td>fcc</td>
<td>0.198</td>
<td>0.561</td>
<td>0.217</td>
<td>0.061</td>
</tr>
<tr>
<td>( d = 4 ) hypercube</td>
<td>0.197</td>
<td>0.573</td>
<td>0.255</td>
<td>0.073</td>
</tr>
<tr>
<td>( d = \infty ) hypercube</td>
<td>0</td>
<td>0.5</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2. Same as table 1 except for site percolation.

which is a little different from (19). The vector \(|s\rangle\) varies depending on the defect and the direction of the strain. For the strain in the triangular net, shown in figure 2

\[
|s\rangle = (d)^{1/2} \begin{pmatrix}
1 \\
1/2 \\
-1/2 \\
-1 \\
-1/2 \\
1/2
\end{pmatrix}
\]  

(42)

Fortunately, we shall not need to write \(|s\rangle\) in detail. A little thought will convince the reader that, for any \(|s\rangle\) derived from (39)

\[
\mathbf{V}|s\rangle = (\alpha_0 - a)|s\rangle
\]  

(43)

which differs from (20) by a factor of 2, because each atom in the shell connects only to the stationary centre in this case. Hence

\[
\Delta E = (-z/2d)\varepsilon^2 a^2 \{(\alpha_0 - a)/[1 - (\alpha_0 - a)(s|\mathbf{P}|s)]\}
\]  

(44)

where we again use the fact that \(|s\rangle\) is an eigenstate of \( \mathbf{P} \). The argument in this case is a little more subtle. The state vector \(|s\rangle\) transforms as a vector on the shell of the defect. As \( \mathbf{P} \) is a scalar under transformations, and there is only single-vector representation on the shell, the result follows.
Combining (38) and (44), we see that

\[ E + \Delta E = \frac{4e^2 N\alpha}{d}[\alpha - 2c(\alpha_0 - \alpha)/[1 - (\alpha_0 - \alpha)(s|P|s)]] \] (45)

The factor 2 in the numerator occurs because of the counting and comes about because a bond is removed if either of the two sites at its end is removed. From (28) we can define \( \alpha_e \) as

\[ \alpha_e = 1 - 2c(\alpha_0 - \alpha)/[1 - (\alpha_0 - \alpha)(s|P|s)] \] (46)

Inverting to first order in \( c \), we have

\[ \alpha_e = \alpha + 2c(\alpha_0 - \alpha)/[1 - (\alpha_0 - \alpha)(s|P|s)] \] (46a)

Note how the factors 2 occur differently in (30a) and (46). The problem is now reduced to evaluating \( \langle s|P|s \rangle \). The components of \( |s \rangle \) are just proportional to \( \delta_i \cdot \delta \) as seen, for example, in (42). If normalised properly to 1, they become \( (d/z)^{1/2} (\delta_i \cdot \delta)/a \).

Therefore

\[ \langle s|P|s \rangle = -\frac{d}{Nza^2} \sum_k (\delta_i \cdot \delta) \exp(ik \cdot \delta) \exp(ik \cdot \delta) \] (47)

where

\[ \nabla = \left( \frac{\partial}{\partial(k,\alpha)} \right) \] (48)

and it is convenient to include the nearest-neighbour distance \( a \) in the definition of the \( \nabla \) operator. For the special case of a missing site, \( \alpha_0 = 0 \) and \( \alpha_e \) extrapolates to zero at

\[ p_1 = \frac{1}{2} - \frac{1}{2} \alpha \langle s|P|s \rangle \] (49)

\[ = \frac{1}{2} + \frac{1}{2N} \sum_k \frac{(\nabla \gamma_k)^2}{1 - \gamma_k} \] (49a)

These integrals for \( p_1 \) have to be computed numerically in most cases. They are listed for a number of lattices in Table 2. The square net has

\[ \gamma_k = \frac{1}{2}(\cos k_x a + \cos k_y a) \]

and so

\[ p_1 = \frac{1}{2} + \frac{1}{8N} \sum_k \frac{2 - \cos 2k_x a - \cos 2k_y a}{2 - \cos k_x a - \cos k_y a} \]

\[ = \frac{1}{2} + \frac{1}{8\pi^2} \int_0^\pi \int_0^\pi \frac{(2 - \cos 2x - \cos 2y)}{2 - \cos x - \cos y} \, dx \, dy \]

\[ = 1 - 1/\pi \]

as previously found by Watson and Leath (1974). The result for the simple cubic lattice was first obtained by Izyumov (1966) in the slightly more complex situation involving spins. His result agrees with ours.
Equation (33) still holds for the site vacancy of course where now
\[ P_c = 1 - c + O(c^2) \]  
(50)
as removing a single site reduces the number of sites in the infinite cluster. Hence \( G \) has a different initial slope from \( D \). Using (33)
\[ 1 - c/(1 - p_1) = (1 - c) [1 - c/(1 - p'_1)] \]
and hence
\[ p'_1 = 2 - 1/p_1. \]  
(51)
These values are also listed in table 2. The results of computer simulations for \( G \) and \( p_s \) (and hence \( D \)) for site percolation on the triangular net are shown in figure 3 (Tang 1986). The broken lines corresponding to the intercepts \( p_i \) and \( p'_1 \) from table 2 are shown. The diffusion constant \( D \) was obtained in figure 3 using (33).

![Figure 3. D (■), P (△) and G (+) for site percolation on the triangular net obtained numerically (Tang 1986) using methods similar to those described by Kirkpatrick (1973). Each sample contained 1600 atoms and the results were averaged over 20 samples. The quantities \( p_i \) and \( p'_1 \) where the initial slopes cross the abscissa are indicated.](image)

5. Comments

We have shown how a number of known results can be put together. Although we have concentrated on bond and site vacancies, knowledge of \( p_i \) allows \( \alpha_c \) to be found for any defect that has a strength \( \alpha_0 \) in a host \( \alpha \). For a bond, using (30a) and (32a),
\[ \alpha_c = \alpha + ca(\alpha_0 - \alpha)/[\alpha(1 - p_1) + \alpha_0 p_1] \]  
(52)
while, using (46a) and (49), for a site defect
\[ \alpha_c = \alpha + 2ca(\alpha_0 - \alpha)/[2\alpha(1 - p_1) + \alpha_0(2p_1 - 1)] \]  
(53)
Isolated defects in the static limit

where in both cases $p_1$ can be looked up in tables 1 or 2. For example these can be used in the 'superconducting limit' (Straley 1983) when $\alpha_0 \to \infty$, to give

$$\alpha_e = \alpha + c\alpha/p_1$$

(52a)
in the bond case and

$$\alpha_e = \alpha + 2c\alpha/(2p_1 - 1)$$

(53a)
in the site case. It is more usual to write these results in terms of the inverses, which to first order in $c$ are

$$1/\alpha_e = (1/\alpha)(1 - c/p_1)$$

(52b)

and

$$1/\alpha_e = (1/\alpha)[1 - 2c/(2p_1 - 1)].$$

(53b)

From (52b) and (53b), we can determine a new quantity $p_1$ for the superconducting limit where the initial slope crosses the abscissa. This is clearly simply related to $p_1$ for the dilute-resistor network on the same lattice. It is more usual to introduce a fraction $p$ of superconducting links so that both problems have a common $p_e$ as sketched in figure 4. This can be imagined as follows. Take a resistor network with a fraction $p$ of bonds

![Figure 4. A sketch of the conductance G versus p showing the intercept $p_1$ of the initial slope. This network has a fraction $p$ of missing units (sites or bonds). Also shown is a sketch of the resistance R versus p, the superconducting limit, showing the intercept $p_1$ of the initial slope. This network has a fraction 1 − p of superconducting bonds. Both G and R are normalised to the same quantity in the respective pure systems.](image)

having a resistance $R_1$ and a fraction $1 - p$ having $R_2$ with $R_2 \gg R_1$. The dilute-resistor limit is reached as $R_2 \to \infty$, whilst the superconducting limit is reached when $R_1 \to 0$. A similar situation holds for site percolation. Therefore, using (52b) and (53b) and remembering to put $p \to 1 - p$ for the superconducting case, we find that for bonds

$$p_1^t = p_1$$

(54)

whilst for sites

$$p_1^s = p_1 - \frac{1}{2}. $$

(55)
Again, like equations (35) and (51) relating \( p_1 \) to \( p_t \), equations (54) and (55) do not depend on the lattice or the dimensionality. Note that \( p_1 \) for sites is given from (49a) and (55) as

\[
p_1^s = \frac{1}{2N} \sum_k \left( \frac{\nabla \gamma_k}{1 - \gamma_k} \right)^2.
\] (55a)

We note that, if the defects are sufficiently far apart, it is \( 1/\alpha_c \) (or the resistance) that is linear in \( c \), the concentration of defects, and contains no \( c^2 \) terms. The \( c^2 \) terms therefore would represent interactions between defects. However, \( \alpha_c \) (or the conductivity) is also linear in \( c \) but contains terms in \( c^2 \) even if the defects are sufficiently far apart that they do not interact. These come purely from the expansion of the denominator, i.e.

\[
[1 + c/(1 - p_1)]^{-1} = 1 - c/(1 - p_1) + O(c^2).
\] (55b)

This is rather obvious but we have not been aware of it before.

Throughout this paper we have used the quantity \( p_1 \), which is where the initial slope, when extrapolated, crosses the horizontal axis. This is a useful way to parametrise the initial slope. Comparing \( p_1 \) and \( p_c \) gives some idea of how close to linear the conductivity is for all \( p \). For example the conductivity is close to linear for most of the range for bond percolation on the square net \( (p_t = p_c = \frac{1}{2}) \) but very far from linear for site percolation on the FCC lattice \( (p_t = 0.198 \text{ and } p_t = 0.561) \) (see tables 1 and 2 and also Kirkpatrick (1973)).

Finally we comment on the spin-wave stiffness. Consider a Heisenberg ferromagnet with spins \( S \) coupled by nearest-neighbour exchange \( J \) and introduce a few isolated site impurities \( S' \) that are coupled to their neighbours with exchange \( J' \). Izumov (1966) calculated the spin-wave stiffness \( D_1 \) by looking at long wavelengths when the excitation energies \( E_k \) are given by \( E_k = D_1 k^2 \). This is a dynamic calculation which is technically rather harder than the static strain calculations done in this paper. Izumov's result for \( D_1 \) (again in units where \( D_1 = 1 \), when \( p = 1 \)) is

\[
D_1 = 1 - c[\delta - 1 - 2\rho/(1 + \Lambda\rho)]
\] (56)

where

\[
\delta = S'/S
\] (57)

\[
\rho = J'S'/JS - 1
\]

and \( \Lambda \) is a number that is given as a lattice integral over the cubic Brillouin zone. Using (33), we can identify

\[
G = 1 + 2c\rho/(1 + \Lambda\rho)
\] (58)

and

\[
P_s = 1 + c(\delta - 1).
\] (59)

The quantity (58) reduces to our \( G \) or \( \alpha_c \) in equation (46) if we put \( S = S' \) (to obtain the usual tight-binding model) and identify \( \rho = J'/J - 1 = \alpha_0/\alpha - 1 \) and also use in (49)

\[
p_t = (1 + \Lambda)/2.
\] (60)

We have checked equation (60) for the simple cubic lattice using our expression for \( p_t \) and the expression given by Izumov for \( \Lambda \) and shown that the two lattice integrals are identically the same.
We therefore conclude that the spin-wave stiffness (56) of Izyumov can be used for any of the lattices in table 2, if \( \Lambda = 2p_1 - 1 \) is used. This may surprise the reader familiar with the intricacies of Izyumov’s paper which seem to be very dependent on the simple cubic lattice. The work here shows that is not so and the result (56) only depends on the lattice through \( \Lambda \).

The inertia term (59) reduces to the usual \( P_s \) given in (50) if \( S' = 0 \), when the central spin plays no role in the dynamics. For a mass defect \( m' \) in a host with masses \( m \)

\[
P_s = 1 + c(m'/m - 1)
\]

which is proportional to the total mass of the system. As long as the impurity mass \( m \) is coupled into the lattice, (61) is the correct expression. As soon as \( \alpha_0 = 0 \), however, \( m' \) is irrelevant in the propagation of sound waves and therefore should be set equal to zero, hence recovering (50). This is also the case in the spin-wave result (56) where \( S' \) should be set equal to zero (i.e. \( \delta = S'/S = 0 \)) if \( J' = 0 \), as the central spin is decoupled from the rest of the lattice and so should not contribute to the inertia term (59) for the propagation of spin waves.

If we return to the original isotropic Born model, we may combine (53) and (61) using (36) to give the velocity \( \nu_s \) of sound for a small concentration of site defects as

\[
mv_s^2 = \frac{za^2}{2d} \left( \alpha + \frac{2ca(\alpha_0 - \alpha)}{2a(1 - p_1) + \alpha_0(2p_1 - 1)} \right) \left[ 1 + c(m'/m - 1) \right]
\]

where the \( p_1 \) are given in table 2.

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Appendix

The general result for the effective \( \alpha_e \) due to the presence of a defect is

\[
\alpha/\alpha_e = 1 - u_0 \cdot T \cdot u_0/u_0 \cdot D_0 \cdot u_0
\]

where \( u_0 \) is the strain in the system before the defect is added. Although (29) was derived with a local defect in mind, it is quite generally true for any change \( V \) in the dynamical matrix. We give two simple illustrations of the use of (29).

In the first we suppose that all the bonds in a system described by (13) have their force constants changed from \( \alpha \) to \( \alpha_0 \). This is not a localised defect, but (29) is general for any \( V \). In this case,

\[
V = [(\alpha_0 - \alpha)/\alpha]D_0
\]

and hence

\[
T = V[1 - P[(\alpha_0 - \alpha)/\alpha]D_0]^{-1} = V[1 + (\alpha_0 - \alpha)/\alpha]^{-1} = (\alpha/\alpha_0)V
\]
where we have used \( \mathbf{PD} = -1 \). Therefore, we have

\[
\frac{\alpha}{\alpha_c} = 1 - (\mathbf{u}_0 \cdot (\alpha \mathbf{V}/\alpha_0) \cdot \mathbf{u}_0)/(\mathbf{u}_0 \cdot \mathbf{D}_0 \cdot \mathbf{u}_0) = 1 - (\alpha/\alpha_0)([\alpha_0 - \alpha]/\alpha) = \alpha/\alpha_0 \tag{A3}
\]

which gives the expected result \( \alpha_c = \alpha_0 \).

In the second example, we consider a 1D chain described by (13) in which a single bond is changed from \( \alpha \) to \( \alpha_0 \).

Equation (30) becomes (with \( c = 1/N \) and \( z = 2 \))

\[
\frac{\alpha}{\alpha_c} = 1 - (1/N)(\alpha_0 - \alpha)/(1 + (\alpha_0 - \alpha)/\alpha) \\
= 1 - (1/N)(\alpha_0 - \alpha)/\alpha_0 \tag{A4}
\]

which can be rewritten as

\[
\frac{N}{\alpha_c} = (N - 1)/\alpha + 1/\alpha_0 \tag{A5}
\]

which is the expected result for \( N - 1 \) spring \( \alpha \) and one spring \( \alpha_0 \) in series.

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