and has the value 0.282. This justifies the exclusion of the interactions of the third nearest neighbors of the second (nonequivalent) type, viz., those of the $P$ atoms. In view of the smallness of the magnitude of the out-of-plane bending constant $\kappa(=0.078)$ of the $I$ atoms, the out-of-plane bending constant $\kappa'$ of the $N$ atoms is not taken into account. SOE constants and the experimental limiting frequencies are to be used to fix the second-order parameters. In the case of titanium the experimental dispersion relations are not available, while the same are present for zirconium.[6] The lattice dynamics, TOE constants, and thermal expansion of zirconium have been worked out by Menon and Rao[12] and the second-order parameters of zirconium have been used as a guideline in fitting up the nine second-order parameters for titanium. Another point that may be noted here is that the third-order parameters $\eta$ and $\chi$ of the $N$ and $K$ atoms, respectively, have also been included to get a better agreement with the experimental results on thermal expansion and the pressure derivatives of the SOE constants of these two metals. In titanium we notice anisotropy even in the basal plane as $C_{111}$ and $C_{222}$ differ from each other considerably. For the time being the discrepancy between $\bar{\gamma}_H$ calculated from the hydrostatic pressure derivatives of the SOE constants of titanium and $\bar{\gamma}_H(\alpha_V)$ calculated from the thermal-expansion data appears to be unresolved. The phonon-dispersion relations are essentially similar to those in zirconium.[6]

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# Integral Methods in the Calculation of Correlation Factors in Diffusion*

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Correlation factors are calculated for vacancy motion over various anisotropic lattices. The calculations exploit the relationship between diffusion and generalized random walks over related lattices, and thus involve the Green's functions for these lattices. Tables of the Green's functions for anisotropic cubic lattices are given.

## I. INTRODUCTION

Correlation factors were introduced into considerations of diffusion mechanisms by Bardeen and Herring[1] in 1952 as the ratio of the diffusion coefficient of a species to the diffusion coefficient of that species computed on the assumption of randomly oriented jump vectors. In general, the correlation factors so defined are less than unity, for successive jumps of a diffusing particle tend to be in opposite directions, as is obvious where diffusion is via a vacancy mechanism. In passing,

it may be remarked that it is surprising that correlation factors were not introduced earlier since, in a sense, they are the result of an effect converse to the "persistence of velocity," which was known in the kinetic theory of gases from the time of Maxwell.[2]

Recently, much effort, both experimental and theoretical, has been expended in determining correlation factors for various types of diffusion in different classes of crystals. The object of these investigations is twofold: If the diffusion mechanism is known, comparison of measured and calculated values of the correlation factor enables one to deduce values for certain atomic parameters; if the diffusion mechanism is not known, an accurate measurement of the correlation factor may make it possible to decide between two alternative mechanisms. These matters, together with other pertinent information about diffusion mechanisms, have been reviewed by Manning[3] and are not discussed further here.

A general formula for the correlation factor has been given by Howard[4]:

$$f = 1 + 2\underline{b} \cdot \underline{T}(\underline{I} - \underline{T})^{-1} \cdot \underline{d} \,, \tag{1.1}$$

where $f$ is the correlation factor, $\underline{b}$ is a row-matrix giving the fractions of jumps of various types, $\underline{T}$ is a square matrix made up of elements that are related to the probabilities of succession of jumps of various types (these matrix elements will be discussed below), $\underline{I}$ is the unit matrix, and $\underline{d}$ is a column matrix giving the projections of the jump lengths on a chosen axis. This formula is derived subject to the usual restrictions of the random-walk formulation. These do not appear to be serious in most cases of physical interest. In Eq. (1.1) the factors $\underline{b}$ and $\underline{d}$ are easily evaluated by inspection, but the determination of the elements of the matrix $\underline{T}$ is often a difficult task. It is precisely this point that we wish to discuss in this paper. Most of the previous calculations of correlation factors have been carried out for various lattices for which the matrix $\underline{T}$ is simply a number (i.e., the average value of the cosine of the angle between successive jumps) and we illustrate our method by considering these relatively simple cases first.

## II. PLANAR LATTICES

Consider the triangular lattice of Fig. 1, which depicts the situation existing immediately after the tracer has jumped from the site marked 0, which is now occupied by the vacancy. The sites are labeled as neighbors to the vacancy site. There is obviously only one type of jump in this lattice (the one just described) and Eq. (1.1) reduces to

$$f = (1+t)/(1-t) \,, \tag{2.1}$$

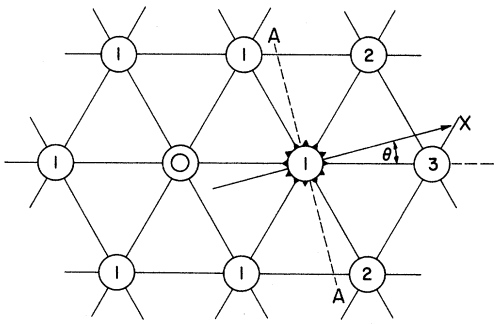


FIG. 1. Vacancy motion in the triangular lattice.

where $t$ is the lone matrix element. In Fig. 1, the direction along which diffusion is measured is designated by $x$, and the line perpendicular to $x$ by $A$-$A$. The quantity $t$ is then given by the product of the probability that the tracer will jump to a nearest-neighbor site and the *expectation* that the vacancy will be at that site multiplied by a projection of that jump on $x$. Note that if we choose $\theta = 30°$, the jumps to sites 1 and 2 (near the $A$'s) are perpendicular to $x$, and hence have zero projections, and we can write

$$t = \tfrac{1}{6}[-F(0) - F(1) + F(2) + F(3)] \,, \tag{2.2}$$

where $\frac{1}{6}$ is the probability of jumping to any given nearest neighbor and $F(k)$ is the expectation that the vacancy is at site $k$. Furthermore, the projections of the jumps are of equal magnitude.

Although it is convenient to choose $\theta = 30°$, it is not necessary to do so. For an arbitrary $\theta$,

$$\begin{aligned} t &\sim \tfrac{1}{6}\{-F(0)\cos\theta - F(1)[\sin(30°-\theta) + \cos(60°-\theta)] \\ &\quad + F(2)[\cos(60°-\theta) + \sin(30°-\theta)] + F(3)\cos\theta\} \\ &\sim \tfrac{1}{6}\left[-F(0) - F(1)\left(\frac{\sin(30°-\theta) + \cos(60°-\theta)}{\cos\theta}\right)\right. \\ &\quad \left. + F(2)\left(\frac{\cos(60°-\theta) + \sin(30°-\theta)}{\cos\theta}\right) + F(3)\right] \\ &= \tfrac{1}{6}[-F(0) - F(1) + F(2) + F(3)] \,, \end{aligned} \tag{2.3}$$

so that the same expression is obtained if all projections are defined relative to that of $F(0)$, which we normalize to unity. This independence of angle occurs whenever diffusion is isotropic and may be used as a test for isotropy.

It now remains to calculate the expectation values. These are calculated on the basis of the *vacancy* making a random walk, with *only* nearest-neighbor jumps, over the given lattice. It has been pointed out[5] that (physically) the walk can be considered to be random only if the atomic array relaxes to its equilbrium configuration in a time short compared to the time between jumps. In the

following it is assumed that this condition is met. For a few simple lattices, there exist analytical solutions for such random walks, which we shall exploit. For more complicated lattices, the *difference equations* describing the walk must be solved by some approximate scheme. In the case of two-dimensional lattices, such as we are now considering, it can be shown[6] that the expectation values in Eq. (2.3) all become infinite for a lattice of infinite extent. This difficulty may be overcome by defining, for a finite lattice, the quantities

$$G(k)=F(0)-F(k)\ , \tag{2.4}$$

which remain finite as the boundaries of the lattice recede to infinity. In terms of these quantities, $t$ for the triangular lattice is

$$t=\tfrac{1}{6}[G(1)-G(2)-G(3)]\ . \tag{2.5}$$

These quantities have been evaluated[7] analytically and it is found that

$$\begin{aligned} t&=\tfrac{1}{6}[1-(6\sqrt{3}/\pi-2)-(8-12\sqrt{3}/\pi)]\\ &=\sqrt{3}/\pi-\tfrac{5}{6}=-0.282\,004\,45\ldots \end{aligned} \tag{2.6}$$

and

$$f=(\pi+6\sqrt{3})/(11\pi-6\sqrt{3})=0.560\,057\,06\ldots\ .$$

These values agree to five figures with those given by Compaan and Haven[8] and with the exact values determined combinatorially by Schoen and Lowen.[9]

For the simple quadratic lattice it is easily shown that

$$\begin{aligned} t&=\tfrac{1}{4}[-F(0)+F(3)]=-\tfrac{1}{4}G(3)\\ &=-\tfrac{1}{4}(4-8/\pi)=-0.363\,380\,23\ldots \end{aligned} \tag{2.7}$$

and

$$f=1/(\pi-1)=0.466\,942\,19\ldots\ ,$$

where the exact value of $G(3)$ is taken from McCrea and Whipple.[10] Again, these values agree with those previously reported.[8,9]

The situation in the honeycomb lattice is illustrated in Fig. 2, from which it is easily seen that

$$t=\tfrac{1}{3}[-F(0)+F(2)]\ . \tag{2.8}$$

This lattice is so open that $F(2)$ may be written as a function of $F(0)$ $[F(2)=F(0)-\frac{3}{2}]$ immediately from the difference equations, so that

$$t=-\tfrac{1}{2},\quad f=\tfrac{1}{3}\ .$$

Similar considerations apply to the diamond lattice where it is easy to show

$$\begin{aligned} &t=\tfrac{1}{4}[-F(0)+F(2)]\ ,\\ &F(2)=F(0)-\tfrac{4}{3}\ ,\\ &t=-\tfrac{1}{3},\quad f=\tfrac{1}{2}\ . \end{aligned} \tag{2.9}$$

In fact, this may be extended to $n$ dimensions if

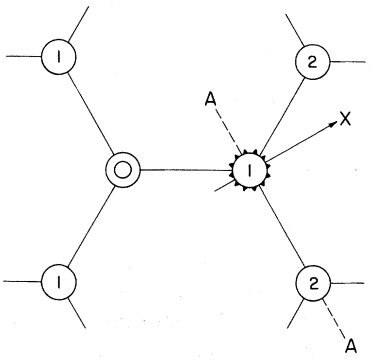


FIG. 2. Vacancy motion in the honeycomb lattice.

$z$, the number of nearest neighbors, can be determined, for obviously

$$f=(z-2)/z\ .$$

For example, if $n=4$ the most open lattice is that formed by placing a point in the center of a pentahedron and its neighbors at the five corners; hence, $z=5$, and $f=\frac{3}{5}$. Incidentally, the formula $f=1-2/z$ is often used to estimate $f$, and we see this is equivalent to replacing the given lattice (fcc, say) with the most open lattice having the same number of nearest neighbors.

## III. CUBIC LATTICES

In considering diffusion in cubic lattices it is possible to use the simple relation (2.1) because all jumps are of the same type. For the simple cubic (sc) lattice, it is easy to see that

$$t=\tfrac{1}{6}[-F(0)+F(4)]\ . \tag{3.1}$$

The expectation values are found by solving the difference equation

$$\begin{aligned} F(u,v,w)=\delta_{u0}\delta_{v0}\delta_{w0}+\tfrac{1}{6}[&F(u-1,v,w)+F(u+1,v,w)\\ &+F(u,v-1,w)+F(u,v+1,w)\\ &+F(u,v,w-1)+F(u,v,w+1)]\ , \end{aligned} \tag{3.2}$$

where the vacancy has been placed at the origin (0, 0, 0) and $u$, $v$, and $w$ are the ordinary Cartesian coordinates. McCrea and Whipple[10] have shown that (3.2), for an infinite lattice, is satisfied by the integral

$$F(u,v,w)=\frac{3}{\pi^2}\int_0^\pi\int_0^\pi d\alpha d\beta\ \frac{\cos u\alpha\cos v\beta e^{-|w|\gamma}}{\sinh\gamma} \tag{3.3}$$

if

$$\cos\alpha+\cos\beta+\cosh\gamma=3\ .$$

It is thus only necessary to identify $F(4)$ with $F(2,0,0)$ [or $F(0,2,0)$ or $F(0,0,2)$] in order to use their results in (3.1).

Unfortunately, only $F(0,0,0)$ can be evaluated exactly. The other integrals must be approximated numerically. These have been tabulated to six-figure accuracy by Maradudin *et al.*,[11] from whom it is found

$$t = \tfrac{1}{6}(-1.516\,386 + 0.257\,336) = -0.209\,842\,,$$

$$f = 0.653\,109\,.$$

These values agree to the accuracy of their calculations with those given previously.[8,9]

The body-centered cubic (bcc) lattice is somewhat more difficult to visualize, and the situation immediately after a tracer-vacancy exchange is shown, in projection, in Fig. 3. The circles indicate those neighbors to the vacancy that lie in the even planes $(0, \pm 2, \pm 4, \ldots)$ and the squares those neighbors that lie in odd planes $(\pm 1, \pm 3, \ldots)$; the first number identifies the neighbor in the nearest plane, the second number that in the next nearest plane. For example, the vacancy has four third neighbors (only one is shown) in its plane and eight third neighbors (four are shown) in the second planes above and below its plane. From Fig. 3 it is seen that

$$t = \tfrac{1}{8}[-F(0) - F(2) + F(3) + F(5)]\,, \tag{3.4}$$

where an analysis similar to that of McCrea and Whipple shows that the expectation values may be written in the form

$$F(u,v,w) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos u\alpha\,\cos v\beta\, e^{-|w|\gamma}\,d\alpha\,d\beta}{\cos\alpha\,\cos\beta\,\sinh\gamma}\,, \tag{3.5}$$

with

$$\cosh\gamma = (\cos\alpha\,\cos\beta)^{-1}$$

or

$$F(u,v,w) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos u\alpha\,\cos v\beta\, e^{-|w|\gamma}\,d\alpha d\beta}{(1-\cos^2\alpha\,\cos^2\beta)^{1/2}}\,.$$

Of the integrals in (3.4), only $F(0) \equiv F(0,0,0)$ is known. This has been evaluated by Watson[12] to be

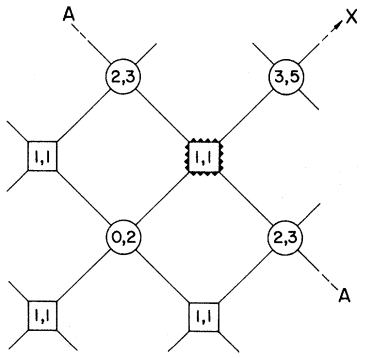


FIG. 3. Vacancy motion in the bcc lattice.

$$F(0,0,0) = (4/\pi^2)K^2(1/\sqrt{2}) \equiv (4/\pi^2)K_0^2\,,$$

where $K(x)$ is the complete elliptic integral of the first kind. By exceedingly good luck, however, it is possible to reduce (3.4) to one integral that can be evaluated. The procedure is as follows: The difference equations for $F(0)$ and $F(1)$ yield

$$F(5) = 7F(0) - 8 - 3F(2) - 3F(3)\,,$$

so that

$$t = \tfrac{1}{8}[-8 + 6F(0) - 4F(2) - 2F(3)]\,. \tag{3.6}$$

The analytical forms for $F(2)[F(2,0,0)]$ and $F(3)[F(2,2,0)]$ may be converted to

$$F(2) = -F(0) + \frac{2}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos^2\alpha\,d\alpha d\beta}{(1-\cos^2\alpha\,\cos^2\beta)^{1/2}}\,,$$

$$F(3) = F(0) - \frac{4}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos^2\alpha\,d\alpha d\beta}{(1-\cos^2\alpha\,\cos^2\beta)^{1/2}} + \frac{4}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos^2\alpha\,\cos^2\beta\,d\alpha d\beta}{(1-\cos^2\alpha\,\cos^2\beta)^{1/2}}\,,$$

and

$$t = \frac{1}{8}\left(-8 + 8F(0) - \frac{8}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos^2\alpha\,\cos^2\beta\,d\alpha d\beta}{(1-\cos^2\alpha\,\cos^2\beta)^{1/2}}\right)$$

$$= -1 + \frac{1}{\pi^2}\int_0^\pi\int_0^\pi (1-\cos^2\alpha\,\cos^2\beta)^{1/2}\,d\alpha d\beta\,. \tag{3.7}$$

The integral, in its final form, has been evaluated by Kaplan[13] as

$$\int_0^\pi\int_0^\pi (1-\cos^2\alpha\,\cos^2\beta)^{1/2}\,d\alpha\,d\beta = 2K_0^2 + \pi/2K_0^2\,, \tag{3.8}$$

whence

$$t = -1 + (2/\pi^2)K_0^2 - \tfrac{1}{2}K_0^{-2} = -0.157\,947\,42\ldots$$

and

$$f = 0.727\,194\,14\,.$$

The value of $t$ agrees with that given by Schoen and Lowen.[9] The two forms are connected by the Legendre relation.[14] These results, together with some additional integrals by Kaplan[13] and the difference equations for the bcc lattice, make possible the exact evaluation of many of the expectation values (Green's functions) for the bcc lattice. The details are given in Appendix A.

In considering the fcc lattice it would appear to be wise to choose the direction of diffusion in such a way that the plane perpendicular to that direction contains as many nearest neighbors of the tracer as possible, i.e., is a closest-packed plane. The lattice projected on this plane is shown in Fig. 4, where the direction of diffusion is out of the paper. Again the circles represent sites in planes equivalent to that containing the vacancy (say, $a$ planes); the squares represent sites in planes (say, $b$ planes), one above and two below the chosen plane.

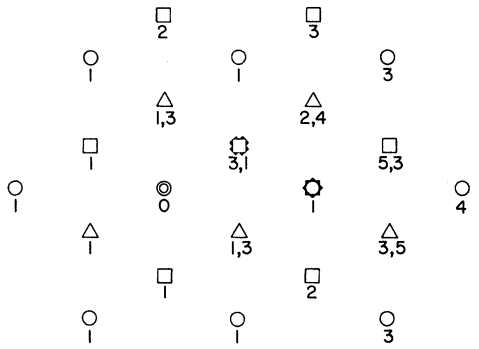


FIG. 4. Vacancy motion in the fcc lattice.

The triangles represent sites in planes ( $c$ planes), one below and two above the vacancy plane. The numbers near the sites represent neighbors to the vacancy occupying those sites. Two of the possible sites for the tracer are shown. It is easily verified that these yield the same expression for $t$, namely,

$$t = \tfrac{1}{12}\left[-F(0) - 2F(1) + 2F(3) + F(4)\right] . \qquad (3.9)$$

Solving the difference equation, which may be written by inspection of Fig. 4, by the method of McCrea and Whipple yields expectation values given by

$$F(u, v, w) = \frac{3}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos u\alpha \cos v\beta e^{-|w|\gamma}\, d\alpha d\beta}{(\cos\alpha + \cos\beta)\sinh\gamma} , \qquad (3.10)$$

with

$$\cosh\gamma = (3 - \cos\alpha\cos\beta)/(\cos\alpha + \cos\beta) .$$

These may be written in the form

$$F(u, v, w) = \frac{3}{\pi^2} \times\int_0^\pi\int_0^\pi \frac{\cos u\alpha\, \cos v\beta e^{-|w|\gamma}\, d\alpha d\beta}{\left[(3 - \cos\alpha\cos\beta)^2 - (\cos\alpha + \cos\beta)^2\right]^{1/2}} .$$

Of the integrals in (3.9), only $F(3)$ contains the exponential term, and it may be eliminated by the difference equations, so that

$$t = \tfrac{1}{12}\left[-3F(0) + 4F(1) - 2F(2) + F(4)\right] . \qquad (3.11)$$

Of these expectation values, $F(0)$ and $F(1)$ are known:

$$F(0) \equiv F(0, 0, 0) = 1.344\,661\,1830\ldots$$

and

$$F(1) \equiv F(1, 1, 0) = F(0) - 1 = 0.344\,661\,1830\ldots$$

from the difference equation for $F(0)$. The other two integrals,

$$F(2) \equiv F(2, 0, 0) = \frac{3}{\pi^2} \times\int_0^\pi\int_0^\pi \frac{\cos 2\alpha\, d\alpha d\beta}{\left[(3 - \cos\alpha\cos\beta)^2 - (\cos\alpha + \cos\beta)^2\right]^{1/2}} ,$$

$$F(4) \equiv F(2, 2, 0) = \frac{3}{\pi^2} \times\int_0^\pi\int_0^\pi \frac{\cos 2\alpha \cos 2\beta\, d\alpha d\beta}{\left[(3 - \cos\alpha\cos\beta)^2 - (\cos\alpha + \cos\beta)^2\right]^{1/2}} ,$$

were evaluated by a computer program utilizing Gaussian quadrature (16 and 24 points) to be

$$F(2) = 0.229\,936\,0607 ,$$

$$F(4) = 0.170\,889\,3539 .$$

[This precision was not sought; it was given with the program, which computed $F(0)$ and $F(1)$ to ten-figure accuracy, so it is assumed that $F(2)$ and $F(4)$ are equally accurate.] Substituting in (3.11) yields

$$t = -0.122\,680\,0660, \qquad f = 0.781\,451\,4220 .$$

The value of $f$ given by Compaan and Haven[8] (0.781 46) is in excellent agreement.

## IV. ANISOTROPIC LATTICES

The simplest extension of the method to anisotropic lattices is to the primitive tetragonal lattice, which is equivalent to a sc lattice with a probability of movement $\nu_a$ in the $xy$, e.g., plane and probability of movement $\nu_c$ perpendicular to that plane. This case was considered by Mullen[15] in his pioneering work on anisotropic lattices. It is, however, not much more difficult to consider the primitive orthorhombic lattice, which we view as equivalent to a sc lattice with probability of movement $\nu_a$ along the $x$ axis, $\nu_b$ along the $y$ axis, and $\nu_c$ along the $c$ axis. Letting

$$\nu_a = \frac{1}{2}\left(\frac{1}{1+\mu+\nu}\right), \quad \nu_b = \frac{1}{2}\left(\frac{\mu}{1+\mu+\nu}\right), \quad \nu_c = \frac{1}{2}\left(\frac{\nu}{1+\mu+\nu}\right),$$

the solution to the random walk of the vacancy may be written as

$$F(u, v, w) = \frac{1+\mu+\nu}{\pi^2} \times\int_0^\pi\int_0^\pi \frac{\cos u\alpha\, \cos v\beta e^{-|w|\gamma}\, d\alpha d\beta}{\nu\sinh\gamma} , \qquad (4.1)$$

with

$$\cos\alpha + \mu\cos\beta + \nu\cosh\gamma = 1 + \mu + \nu .$$

It is evident that the $t$'s are given by

$$t_a = \nu_a\left[-F(0, 0, 0) + F(2, 0, 0)\right] = \frac{-G(2, 0, 0)}{2(1+\mu+\nu)} ,$$

$$t_b = \nu_b[-F(0,0,0)+F(0,2,0)] = \frac{-\mu G(0,2,0)}{2(1+\mu+\nu)}\ , \tag{4.2}$$

$$t_c = \nu_c[-F(0,0,0,)+F(0,0.2)] = \frac{-\nu G(0,0,2)}{2(1+\mu+\nu)}\ ,$$

and Eq. (2.1) applies in all three cases.

The evaluation of these, and related integrals, is discussed in Appendix B, where Table III gives the integrals for selected values for $\mu$ and $\nu$. Use of this table, and Eqs. (4.2) and (2.1), allows the construction of Table I, which gives the correlation factors as functions of $\mu$ and $\nu$. The values corresponding to $\mu$ (or $\nu$) = 1 are those for the primitive tetragonal lattice. Comparison with the values given by Mullen[15] indicates that his results are accurate to about 1%.

The difference equations resulting from a generalization of a random walk on the fcc lattice in which the probability of movement in the $xy$ plane is $\nu_a$, in the $xz$ plane is $\nu_b$, and in the $yz$ plane is $\nu_c$ can also be solved by an extension of the method of McCrea and Whipple. The complete extension given above does not appear to correspond to a lattice representing any physical array of atoms, but there appears to be enough interest in the Green's functions of such a lattice to warrant the presentation of the values of some of the functions of this generalized lattice. These are given in Appendix C.

If we specialize the case above to that in which $\nu_a = \nu_b$, the body-centered tetragonal (bct) lattice is obtained. In Fig. 5 the lattice is shown projected onto this plane. The circles represent the sites

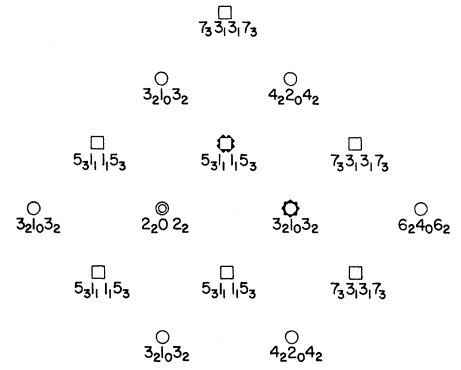

FIG. 5. Vacancy motion in the body-centered-tetragonal lattice.

of atoms in even planes and the squares those of atoms in odd planes. The neighbors occupying such sites are indicated in the figure.

The solution to the difference equation for this walk is

$$F(u,v,w) = \frac{1+2\nu}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos u\alpha\cos v\beta e^{-|w|\gamma}\,d\alpha d\beta}{\nu(\cos\alpha+\cos\beta)\sinh\gamma}\ , \tag{4.3}$$

with

$$\cos\alpha\cos\beta+\nu(\cos\alpha+\cos\beta)\cosh\gamma = 1+2\nu\ ,$$

where $\nu \equiv \nu_c/\nu_a$. The evaluation of these integrals is discussed in Appendix C. They are the integrals listed along the diagonals ($\mu = \nu$) of Table IV.

Now, inspection of Fig. 5 shows that there are two types of jumps, one in the plane occurring with probability $\nu_a$ and one out of the plane with proba-

TABLE I. Correlation factors for primitive orthorhombic lattice.

| $\mu\downarrow$ \ $\nu\rightarrow$ | 0.25 | 0.50 | 0.75 | 1.00 | 1.33··· | 2.00 | 4.00 |
|---|---|---|---|---|---|---|---|
| | | | | $f_a$ | | | |
| 0.25 | 0.414 05 | 0.478 13 | 0.522 06 | 0.555 23 | 0.589 36 | 0.637 78 | 0.716 69 |
| 0.50 | | 0.532 26 | 0.569 99 | 0.598 80 | 0.628 70 | 0.671 55 | 0.742 27 |
| 0.75 | | | 0.603 63 | 0.629 47 | 0.656 44 | 0.695 34 | 0.760 17 |
| 1.00 | | | | 0.653 11 | 0.677 87 | 0.713 73 | 0.773 97 |
| 1.33··· | | $f_a(\mu,\nu) = f_a(\nu,\mu)$ | | | 0.700 36 | 0.733 10 | 0.788 50 |
| 2.00 | | | | | | 0.761 40 | 0.809 78 |
| 4.00 | | | | | | | 0.846 55 |
| | | | | $f_b$ | | | |
| 0.25 | 0.773 97 | 0.809 78 | 0.831 40 | 0.846 55 | 0.861 29 | 0.880 96 | 0.910 55 |
| 0.50 | 0.671 55 | 0.713 73 | 0.741 23 | 0.761 40 | 0.781 69 | 0.809 78 | 0.854 07 |
| 0.75 | 0.604 39 | 0.648 06 | 0.677 87 | 0.700 36 | 0.723 53 | 0.756 43 | 0.810 15 |
| 1.00 | 0.555 23 | 0.598 80 | 0.629 47 | 0.653 11 | 0.677 87 | 0.713 73 | 0.773 97 |
| 1.33··· | 0.505 98 | 0.548 53 | 0.579 38 | 0.603 63 | 0.629 47 | 0.667 69 | 0.733 85 |
| 2.00 | 0.438 30 | 0.478 13 | 0.508 08 | 0.532 26 | 0.558 64 | 0.598 80 | 0.671 55 |
| 4.00 | 0.333 04 | 0.366 08 | 0.392 18 | 0.414 05 | 0.438 75 | 0.478 13 | 0.555 23 |
| | | | | $f_c$ | | | |
| | | | | $f_c(\mu,\nu) = f_b(\nu,\mu)$ | | | |

bility $\nu_c$. For diffusion along the $c$ axis only a type-2 jump is required and we have

$$t_c = \frac{\nu}{4(1+2\nu)} [-F(0) - 2F(1_0) - F(2_0) + F(2_2) + 2F(3_2) + F(4_2)] \quad (4.4)$$

and

$$f_c = (1+t_c)/(1-t_c) . \quad (4.5)$$

For diffusion in the $a$ plane the situation is more complex, however, for here both types of jumps are involved. By inspection, it can be seen that

$$\begin{aligned} t_{11} &= \frac{1}{4(1+2\nu)} [-F(0) + F(4_0)] , \\ t_{12} &= \frac{1}{4(1+2\nu)} [-4\times\tfrac{1}{2}F(1_1) + 4\times\tfrac{1}{2}F(3_1)] \\ &= \frac{\nu}{2(1+2\nu)} [-F(1_1) + F(3_1)] , \\ t_{21} &= \frac{1}{4(1+2\nu)} [-2F(1_1) + 2F(3_1)] \\ &= \frac{1}{2(1+2\nu)} [-F(1_1) + F(3_1)] = \nu^{-1} t_{12} , \\ t_{22} &= \frac{1}{4(1+2\nu)} [-F(0) + F(2_0) - F(2_2) + F(4_2)] . \end{aligned} \quad (4.6)$$

The value of $f_a$ could then be obtained by using Eq. (1.1) (assuming the values of the integrals were known). However, to facilitate comparison with the results of Mullen,[15] we make use of the fact that $t_{11}$ and $t_{12}$ are associated with position $1_0$ and $t_{21}$ and $t_{22}$ with position $1_1$ and define[5]

$$f_a = c_1 f_a(1_0) + c_2 f_a(1_1) , \quad (4.7)$$

where the $c$'s are the fractions of jumps of types 1 and 2, respectively, and

$$\begin{aligned} f_a(1_0) &= \frac{(1+t_{11})(1-t_{22}) + t_{12}(2+t_{21})}{(1-t_{11})(1-t_{22}) - t_{12}t_{21}} , \\ f_a(1_1) &= \frac{(1+t_{22})(1-t_{11}) + t_{21}(2+t_{12})}{(1-t_{11})(1-t_{22}) - t_{12}t_{21}} . \end{aligned} \quad (4.8)$$

The fraction of jumps which are of type 1 is given by

$$\frac{4\nu_a}{4\nu_a + 8\nu_c} = \frac{1}{1+2\nu}$$

and those of type 2 by

$$\frac{8\nu_c}{4\nu_a + 8\nu_c} = \frac{2\nu}{1+2\nu} .$$

The integrals involved in the $t_{ij}$ are expressed in terms of $F(u, v, w)$ as follows:

$$F(0) \equiv F(0,0,0), \quad F(1_0) \equiv F(1,1,0), \quad F(1_1) \equiv F(1,0,1) ,$$
$$F(2_0) \equiv F(2,0,0), \quad F(2_2) \equiv F(2,0,2), \quad F(3_1) \equiv F(2,1,1) ,$$
$$F(3_2) \equiv F(1,1,2), \quad F(4_0) \equiv F(2,2,0), \quad F(4_2) \equiv F(2,0,2) .$$

These can be read from Table IV in Appendix C and the values of $f_a(1_0)$, $f_a(1_1)$, $f_a$, and $f_c$ for some values of $\nu$ are listed in Table II. $f_a(1_0)$ and $f_a(1_1)$ are more accurately defined versions of Mullen's $f_{Ax}$ and $f_{Bx}$ and inspection shows that our results disagree in the third significant figure, again indicating that Mullen's results are good to about 1%.

## V. SUMMARY

It has been shown that correlation factors may be calculated simply and with great accuracy for those lattices for which an analytical solution exists for the expectation that a random walker will visit a given site of the lattice. These solutions can be generalized to encompass anisotropic walks and the correlation factors can be computed as functions of the probabilities of motion in various directions. The expectations of visits in these cases are related to the Green's functions for the lattices and some of the Green's functions for the "anisotropic" cubic lattices have been computed from the integral solutions.

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## APPENDIX A: GREEN'S FUNCTIONS FOR bcc LATTICE

Here we give a brief exposition of the method used to find exact values for the Green's functions for the bcc lattice. The exposition makes use of certain integrals evaluated by Kaplan[13] and the difference equations relating the various functions. The work below should be self-explanatory.

The integrals given by Kaplan are equivalent to

$$\int_0^\pi \int_0^\pi d\alpha d\beta (1 - \cos^2\alpha \cos^2\beta)^{-1/2} = 4K^2(1/2) \equiv 4K_0^2 , \quad (A1)$$

$$\int_0^\pi \int_0^\pi d\alpha d\beta (1 - \cos^2\alpha \cos^2\beta)^{1/2} = 2K_0^2 + \pi^2 (2K_0^2)^{-1} , \quad (A2)$$

$$\int_0^\pi \int_0^\pi d\alpha d\beta \cos^2\alpha (1 - \cos^2\alpha \cos^2\beta)^{-1/2} = 2K_0^2 + \pi^2 (2K_0^2)^{-1} , \quad (A3)$$

$$\int_0^\pi \int_0^\pi d\alpha d\beta \cos^2\alpha (1 - \cos^2\alpha \cos^2\beta)^{1/2} = \tfrac{2}{3} K_0^2 + \pi^2 (2K_0^2)^{-1} , \quad (A4)$$

$$\int_0^\pi \int_0^\pi d\alpha d\beta \cos^2\alpha \cos^2\beta (1 - \cos^2\alpha \cos^2\beta)^{-1/2} = 2K_0^2 - \pi^2 (2K_0^2)^{-1} , \quad (A5)$$

TABLE II. Correlation factors for bct lattice.

| $\nu$ | 0.25 | 0.50 | 0.75 | 1.00 | 1.33··· | 2.00 | 4.00 |
|---|---|---|---|---|---|---|---|
| $f_a(1_0)$ | 0.657 23 | 0.720 34 | 0.757 05 | 0.781 45 | 0.803 85 | 0.831 24 | 0.865 84 |
| $f_a(1_1)$ | 0.856 85 | 0.815 64 | 0.794 52 | 0.781 45 | 0.770 63 | 0.757 63 | 0.743 33 |
| $f_a$ | 0.723 77 | 0.767 99 | 0.779 53 | 0.781 45 | 0.779 69 | 0.772 35 | 0.756 94 |
| $f_c$ | 0.850 78 | 0.813 09 | 0.793 58 | 0.781 45 | 0.772 33 | 0.758 73 | 0.744 43 |

$$\int_0^\pi \int_0^\pi d\alpha d\beta \cos^2\alpha \cos^2\beta (1-\cos^2\alpha\cos^2\beta)^{1/2} = \tfrac{4}{9} K_0^2 . \quad \text{(A6)}$$

The Green's functions, *for* $w=0$, are given by

$$F(u,v,0) = \frac{1}{\pi^2} \times \int_0^\pi \int_0^\pi d\alpha d\beta \cos u\alpha \cos v\beta (1-\cos^2\alpha\cos^2\beta)^{-1/2} . \quad \text{(A7)}$$

The relations among (A7) and the various integrals (A1)–(A6) are obvious[12]:

$$F(0) \equiv F(0,0,0) = \pi^{-2}(\text{A1}) = 4\pi^{-2}K_0^2 = 1.393\,203\,930,$$
$$F(1) \sim F(1,1,1) = F(0) - 1 = 4\pi^{-2}K_0^2 - 1 = 0.393\,203\,930 ,$$
$$F(2) \sim F(2,0,0) = 2\pi^{-2}(\text{A3}) - \pi^{-2}(\text{A1}) = K_0^{-2} = 0.290\,901\,228 ,$$
$$F(3) \sim F(2,2,0) = 4\pi^{-2}(\text{A5}) - 4\pi^{-2}(\text{A3}) + \pi^{-2}(\text{A1}) = 4\pi^{-2}K_0^2 - 4K_0^{-2} = 0.229\,599\,016 ,$$
$$F(4) \sim F(3,1,1) = 2F(2) - F(1) = 1 - 4\pi^{-2}K_0^2 + 2K_0^{-2} = 0.188\,598\,527 ,$$
$$F(5) \sim F(2,2,2) = 8F(1) - F(0) - 3F(2) - 3F(3) = 16\pi^{-2}K_0^2 + 9K_0^{-2} - 8 = 0.190\,926\,774 ,$$
$$F(7) \sim F(3,3,1) = 4F(3) - F(1) - 2F(4) = 20\pi^{-2}K_0^2 - 20K_0^{-2} - 1 = 0.147\,995\,080 ,$$
$$F_1(10) \sim F(3,3,3) = 8F(5) - F(1) - 3F(4) - 3F(7) = 76\pi^{-2}K_0^2 + 126\,K_0^{-2} - 63 = 0.124\,429\,444 .$$

The other Green's functions depend on

$$F(6) \sim F(4,0,0) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi d\alpha d\beta \cos 4\alpha (1-\cos^2\alpha\cos^2\beta)^{-1/2} ,$$

which may be written as

$$F(6) = \frac{8}{\pi^2} \int_0^\pi \int_0^\pi d\alpha d\beta \cos^4\alpha (1-\cos^2\alpha\cos^2\beta)^{-1/2} - 8\pi^{-2}(\text{A3}) + (\text{A1}) .$$

By an extension of the method used by Kaplan, it may be shown that

$$\int_0^\pi \int_0^\pi d\alpha d\beta \cos^4\alpha (1-\cos^2\alpha\cos^2\beta)^{-1/2} = \tfrac{14}{9} K_0^2 + \pi^2 (2K_0^2)^{-1} . \quad \text{(A8)}$$

Therefore,

$$F(6) \sim F(4,0,0) = 8\pi^{-2}(\text{A8}) - 8\pi^{-2}(\text{A3}) + (\text{A1}) = 4(3\pi)^{-2}K_0^2 = 0.154\,800\,437 ,$$
$$F_2(10) \sim F(5,1,1) = 2F(6) - F(4) = 44(3\pi)^{-2}K_0^2 - 2K_0^{-2} - 1 = 0.121\,002\,346 .$$

The Green's function

$$F(8) \sim F(4,2,0) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi d\alpha d\beta \cos 4\alpha \cos 2\beta \times (1-\cos^2\alpha\cos^2\beta)^{-1/2}$$

may be written in terms of known integrals, (A1)–(A8) and

$$\int_0^\pi \int_0^\pi d\alpha d\beta \cos^4\alpha \cos^2\beta (1-\cos^2\alpha\cos^2\beta)^{-1/2} = \tfrac{4}{3} K_0^2 , \quad \text{(A9)}$$

which results from the identity

$$\cos^4\alpha\cos^2\beta(1-\cos^2\alpha\cos^2\beta)^{-1/2} = \cos^2\alpha \times [(1-\cos^2\alpha\cos^2\beta)^{-1/2} - (1-\cos^2\alpha\cos^2\beta)^{1/2}] .$$

Thus,

$$F(8) \sim F(4,2,0) = 16\pi^{-2}(\text{A9}) - 8\pi^{-2}(\text{A8}) - 16\pi^{-2}(\text{A5}) + 10\pi^{-2}(\text{A3}) - \pi^{-2}(\text{A1}) = 9K_0^{-2} - 64(3\pi)^{-2}K_0^2 = 0.141\,304\,070 ,$$
$$F(9) \sim F(4,2,2) = 8F(4) - F(2) - 2F(3) - F(5) - F(6) - 2F(8) = 16 - 380(3\pi)^{-2}K_0^2 - 4K_0^{-2} = 0.130\,353\,606 .$$

This gives all the Green's functions through the first ten neighbor shells, and we do not continue

except to remark that $F(12)$ and $F(15)$ are given by the difference equations as

$$F(12) \sim F(5,3,1) = 4F(8) - F(4) - F(7) - F_2(10)$$
$$= 1 - 444(3\pi)^{-2}K_0^2 + 56K_0^{-2} = 0.107\,620\,325\ ,$$
$$F(15) \sim F(5,3,3) = 8F(9) - F(4) - 2F(7) - F_1(10) - F_2(10) - 2F(12)$$
$$= 191 - 3204(3\pi)^{-2}K_0^2 - 230K_0^{-2} = 0.097\,567\,724\ .$$

All of these values agree with those found independently by Joyce.[16]

## APPENDIX B: GREEN'S FUNCTIONS FOR GENERALIZED sc LATTICE

It is shown in the text that the Green's functions for this lattice may be written in the integral form

$$F(u,v,w) = \frac{1+\mu+\nu}{\pi^2} \times \int_0^\pi \int_0^\pi \frac{d\alpha d\beta \cos u\alpha \cos v\beta e^{-|w|\gamma}}{[(1+\mu+\nu-\cos\alpha-\mu\cos\beta)^2-\nu^2]^{1/2}}\ , \tag{B1}$$

where the exponential term is defined by the auxiliary relation above. If one attempts a numerical evaluation of the integral as it stands, one obtains only three-figure accuracy—even when using Gaussian quadrature with 24 points over the $\beta$ interval and 32 points over the $\alpha$ interval. On the other hand, the related integral

$$G(u,v,w) \equiv F(0,0,0) - F(u,v,w)$$

is given to eight-figure accuracy by this simple procedure. Because the difference integrals $G(u,v,w)$ were needed to calculate the correlation factors, they were evaluated by the procedure above.

In order to obtain the Green's functions from the related integrals it is necessary to obtain $F(0,0,0)$ to comparable accuracy. After applying some transformations that exploit the equivalence of the variables $\alpha$ and $\beta$, it is found that this function may be written as

$$F(0,0,0) = \frac{1+\mu+\nu}{\pi^2} \int_0^\pi d\alpha \times \int_0^\alpha d\beta \{[(1+\mu+\nu-\cos\alpha-\mu\cos\beta)^2-\nu^2]^{-1/2} + [(1+\mu+\nu-\mu\cos\alpha-\cos\beta)^2-\nu^2]^{-1/2}\}\ . \tag{B2}$$

The Gaussian procedure applied to this formula apparently gives ten-figure accuracy—as judged by the fact that it reproduces Watson's value[12] for $\mu=\nu=1$ to that many figures.

The Green's functions for the generalized simple cubic lattice for positions through the fourth neighbor shell are given in Table III. Each part of the table required about 20 sec of computation on the IBM360-75 to evaluate the 49 integrals.

## APPENDIX C: GREEN'S FUNCTIONS FOR GENERALIZED fcc LATTICE

We consider a random walk to nearest neighbors on the fcc lattice of infinite extent with probability of movement in the $xy$ plane given by $\nu_a$, that in the $xz$ plane by $\nu_b$, and that in the $yz$ plane by $\nu_c$, where we must have

$$4\nu_a + 4\nu_b + 4\nu_c = 1\ . \tag{C1}$$

The difference equation defining this walk is

$$F(u,v,w) = \delta_{u0}\delta_{v0}\delta_{w0} + \nu_a[F(u-1,v-1,w)+F(u-1,v+1,w)+F(u+1,v-1,w)+F(u+1,v+1,w)] + \nu_b[F(u-1,v,w-1)+F(u-1,v,w+1)+F(u+1,v,w-1)+F(u+1,v,w+1)] + \nu_c[F(u,v-1,w-1)+F(u,v-1,w+1)+F(u,v+1,w-1)+F(u,v+1,w+1)]\ . \tag{C2}$$

The method of McCrea and Whipple[10] may be applied to show that the solution of the difference equation is given by

$$F(u,v,w) = \frac{1}{\pi^2} \times \int_0^\pi \int_0^\pi d\alpha d\beta\ \frac{\cos u\alpha \cos v\beta e^{-|w|\gamma}}{(4\nu_b\cos\alpha + 4\nu_c\cos\beta)\sinh\gamma}\ , \tag{C3}$$

with

$$4\nu_a\cos\alpha\cos\beta + 4\nu_b\cos\alpha\cosh\gamma + 4\nu_c\cos\beta\cosh\gamma = 1\ .$$

Writing

$$\nu_b/\nu_a \equiv \mu\ ,\quad \nu_c/\nu_a \equiv \nu\ , \tag{C4}$$

and using (C1), we may show that (C3) is equivalent to

$$F(u,v,w) = \frac{1+\mu+\nu}{\pi^2} \times \int_0^\pi \int_0^\pi d\alpha d\beta\ \frac{\cos u\alpha \cos v\beta\, e^{-|w|\gamma}}{(\mu\cos\alpha + \nu\cos\beta)\sinh\gamma}\ , \tag{C5}$$

with

$$\cos\alpha\cos\beta + \mu\cos\alpha\cosh\gamma + \nu\cos\beta\cosh\gamma = 1 + \mu + \nu\ .$$

For $w=0$, this integral may be written in the form

TABLE III. Green's functions for the generalized sc lattice.

| $\mu\downarrow$ $\nu\rightarrow$ | 0.25 | 0.50 | 0.75 | 1.00 | 1.33··· | 2.00 | 4.00 |
|---|---|---|---|---|---|---|---|
| | | | | $F(0,0,0)$ | | | |
| 0.25 | 1.779 444 26 | 1.675 097 40 | 1.661 747 52 | 1.679 001 91 | 1.721 288 45 | 1.831 448 02 | 2.178 170 95 |
| 0.50 | | 1.575 120 36 | 1.554 822 25 | 1.562 481 29 | 1.591 657 57 | 1.675 097 40 | 1.956 523 11 |
| 0.75 | | | 1.525 831 86 | 1.524 926 03 | 1.543 408 67 | 1.607 970 08 | 1.845 919 34 |
| 1.00 | | | | 1.516 386 06 | 1.525 831 86 | 1.575 120 36 | 1.779 444 26 |
| 1.33··· | | $F^{\mu}_{\nu}(0,0,0)=F^{\nu}_{\mu}(0,0,0)$ | | | 1.524 926 03 | 1.557 232 33 | 1.725 407 81 |
| 2.00 | | | | | | 1.562 481 29 | 1.675 097 40 |
| 4.00 | | | | | | | 1.679 001 91 |
| | | | | $F(1,0,0)$ | | | |
| 0.25 | 0.914 907 75 | 0.783 454 84 | 0.735 616 38 | 0.716 228 68 | 0.709 665 45 | 0.723 374 53 | 0.814 294 34 |
| 0.50 | | 0.664 604 80 | 0.617 519 58 | 0.595 489 26 | 0.583 563 68 | 0.584 923 72 | 0.640 561 11 |
| 0.75 | | | 0.568 419 78 | 0.543 682 61 | 0.527 898 47 | 0.521 705 39 | 0.557 911 36 |
| 1.00 | | | | 0.516 386 06 | 0.497 439 92 | 0.485 635 92 | 0.508 517 27 |
| 1.33··· | | $F^{\mu}_{\nu}(1,0,0)=F^{\nu}_{\mu}(1,0,0)$ | | | 0.474 908 47 | 0.457 194 43 | 0.467 017 33 |
| 2.00 | | | | | | 0.430 449 43 | 0.422 014 95 |
| 4.00 | | | | | | | 0.381 187 75 |
| | | | | $F(0,1,0)$ | | | |
| 0.25 | 0.508 517 29 | 0.422 014 97 | 0.392 658 67 | 0.381 187 76 | 0.377 425 55 | 0.385 292 36 | 0.436 016 03 |
| 0.50 | 0.584 923 72 | 0.485 635 93 | 0.447 800 87 | 0.430 449 44 | 0.421 148 98 | 0.422 014 96 | 0.463 229 04 |
| 0.75 | 0.652 951 99 | 0.542 573 41 | 0.497 439 92 | 0.474 908 47 | 0.460 609 84 | 0.454 961 32 | 0.486 875 94 |
| 1.00 | 0.716 228 68 | 0.595 489 26 | 0.543 682 61 | 0.516 386 06 | 0.497 439 92 | 0.485 635 93 | 0.508 517 27 |
| 1.33··· | 0.795 448 75 | 0.661 668 71 | 0.601 615 66 | 0.568 419 77 | 0.543 682 62 | 0.524 123 12 | 0.535 390 62 |
| 2.00 | 0.941 254 23 | 0.783 454 85 | 0.708 480 72 | 0.664 604 81 | 0.629 324 08 | 0.595 489 26 | 0.584 923 72 |
| 4.00 | 1.315 524 79 | 1.097 175 36 | 0.985 241 97 | 0.914 907 76 | 0.853 344 50 | 0.783 454 85 | 0.716 228 69 |
| | | | | $F(0,0,1)$ | | | |
| | | | | $F^{\mu}_{\nu}(0,0,1)=F^{\nu}_{\mu}(0.1,0)$ | | | |
| | | | | $F(1,1,0)$ | | | |
| 0.25 | 0.428 959 49 | 0.349 516 12 | 0.322 890 64 | 0.312 446 99 | 0.308 799 40 | 0.315 028 54 | 0.357 153 35 |
| 0.50 | 0.452 851 51 | 0.364 608 03 | 0.331 752 35 | 0.316 764 53 | 0.308 559 42 | 0.308 340 63 | 0.338 908 29 |
| 0.75 | 0.475 716 22 | 0.379 979 55 | 0.342 097 18 | 0.323 452 05 | 0.311 580 33 | 0.306 200 01 | 0.327 698 50 |
| 1.00 | 0.497 862 23 | 0.395 210 24 | 0.352 942 35 | 0.331 148 61 | 0.316 140 73 | 0.306 378 79 | 0.320 305 25 |
| 1.33··· | 0.526 318 84 | 0.415 055 41 | 0.367 575 16 | 0.342 097 18 | 0.323 452 05 | 0.308 655 20 | 0.314 024 79 |
| 2.00 | 0.579 778 64 | 0.452 851 51 | 0.396 338 84 | 0.364 608 03 | 0.339 872 51 | 0.316 764 53 | 0.308 340 63 |
| 4.00 | 0.718 502 07 | 0.552 679 10 | 0.474 943 17 | 0.428 959 49 | 0.390 656 40 | 0.349 516 12 | 0.312 446 99 |
| | | | | $F(1,0,1)$ | | | |
| | | | | $F^{\mu}_{\nu}(1,0,1)=F^{\nu}_{\mu}(1,1,0)$ | | | |
| | | | | $F(0,1,1)$ | | | |
| 0.25 | 0.320 305 25 | 0.308 340 63 | 0.308 152 02 | 0.312 446 99 | 0.321 214 21 | 0.342 492 58 | 0.408 294 17 |
| 0.50 | | 0.306 378 79 | 0.310 349 94 | 0.316 764 53 | 0.327 019 94 | 0.349 516 12 | 0.415 874 68 |
| 0.75 | | | 0.316 140 72 | 0.323 452 05 | 0.334 256 53 | 0.356 977 32 | 0.422 613 46 |
| 1.00 | | | | 0.331 148 60 | 0.342 097 18 | 0.364 608 03 | 0.428 959 49 |
| 1.33··· | | $F^{\mu}_{\nu}(0,1,1)=F^{\nu}_{\mu}(0,1,1)$ | | | 0.352 942 35 | 0.374 859 29 | 0.437 104 57 |
| 2.00 | | | | | | 0.395 210 23 | 0.452 851 51 |
| 4.00 | | | | | | | 0.497 862 23 |
| | | | | $F(1,1,1)$ | | | |
| 0.25 | 0.300 610 02 | 0.282 194 57 | 0.277 494 31 | 0.278 122 85 | 0.282 728 00 | 0.297 074 13 | 0.347 110 68 |
| 0.50 | | 0.269 762 76 | 0.266 370 21 | 0.266 871 00 | 0.270 511 40 | 0.282 194 57 | 0.324 530 52 |
| 0.75 | | | 0.262 748 39 | 0.262 539 79 | 0.264 998 33 | 0.274 226 96 | 0.310 332 11 |
| 1.00 | | | | 0.261 470 13 | 0.262 748 39 | 0.269 762 76 | 0.300 610 02 |
| 1.33··· | | $F^{\mu}_{\nu}(1,1,1)=F^{\nu}_{\mu}(1,1,1)$ | | | 0.262 539 79 | 0.266 922 67 | 0.291 811 03 |
| 2.00 | | | | | | 0.266 871 00 | 0.282 194 57 |
| 4.00 | | | | | | | 0.278 122 85 |

TABLE III. (*Continued*).

| $\mu\downarrow$ $\nu\rightarrow$ | 0.25 | 0.50 | 0.75 | 1.00 | 1.33··· | 2.00 | 4.00 |
|---|---|---|---|---|---|---|---|
| | | | | $F(2,0,0)$ | | | |
| 0.25 | 0.536 319 50 | 0.439 384 98 | 0.405 698 32 | 0.392 079 21 | 0.386 899 79 | 0.393 857 62 | 0.445 326 49 |
| 0.50 | | 0.354 082 80 | 0.322 294 20 | 0.307 780 01 | 0.299 829 42 | 0.299 621 96 | 0.329 307 90 |
| 0.75 | | | 0.289 975 47 | 0.274 265 58 | 0.264 394 31 | 0.260 165 01 | 0.278 968 30 |
| 1.00 | | | | 0.257 335 90 | 0.245 893 71 | 0.238 777 36 | 0.250 476 67 |
| 1.33··· | | $F_\nu^\mu(2,0,0) = F_\mu^\nu(2,0,0)$ | | | 0.232 658 48 | 0.222 548 89 | 0.227 494 59 |
| 2.00 | | | | | | 0.207 896 80 | 0.203 620 64 |
| 4.00 | | | | | | | 0.183 225 97 |
| | | | | $F(0,2,0)$ | | | |
| 0.25 | 0.250 476 68 | 0.203 620 69 | 0.188 753 88 | 0.183 226 04 | 0.181 659 63 | 0.186 043 83 | 0.211 865 28 |
| 0.50 | 0.299 621 95 | 0.238 777 35 | 0.217 326 40 | 0.207 896 80 | 0.203 020 19 | 0.203 620 67 | 0.224 888 25 |
| 0.75 | 0.346 651 82 | 0.273 539 48 | 0.245 893 69 | 0.232 658 47 | 0.224 479 28 | 0.221 230 79 | 0.237 772 46 |
| 1.00 | 0.392 079 21 | 0.307 780 00 | 0.274 265 56 | 0.257 335 84 | 0.245 893 70 | 0.238 777 36 | 0.250 476 68 |
| 1.33··· | 0.450 641 85 | 0.352 586 37 | 0.311 662 41 | 0.289 975 46 | 0.274 265 56 | 0.262 007 27 | 0.267 138 50 |
| 2.00 | 0.562 226 45 | 0.439 384 99 | 0.384 760 78 | 0.354 082 79 | 0.330 153 79 | 0.307 780 00 | 0.299 621 96 |
| 4.00 | 0.864 793 83 | 0.680 400 95 | 0.590 699 71 | 0.536 319 53 | 0.490 118 52 | 0.439 384 99 | 0.392 079 22 |
| | | | | $F(0,0,2)$ | | | |
| | | | | $F_\nu^\mu(0,0,2) = F_\mu^\nu(0,2,0)$ | | | |

$$F(u,v,0) = \frac{1+\mu+\nu}{\pi^2} \int_0^\pi \int_0^\pi d\alpha d\beta \times \frac{\cos u\alpha \cos v\beta}{[(1+\mu+\nu-\cos\alpha\cos\beta)^2 - (\mu\cos\alpha+\nu\cos\beta)^2]^{1/2}} . \quad \text{(C6)}$$

Attempts to evaluate numerically the integral in this form yielded only three-place accuracy, and the modification used in Appendix B (to write the integral over $\beta$ from 0 to $\alpha$ and to interchange $\alpha$ and $\beta$ in the integrand) increased the accuracy to only four places.

By examining the detailed behavior over the integrand over the region of integration it is seen that (C6) may be written in the form

$$F(u,v,w) = \frac{1+\mu+\nu}{\pi^2} \int_0^{\pi/2} d\alpha \int_0^\alpha d\beta \left( \frac{[1+(-1)^{u+v}]\cos u\alpha \cos v\beta}{(T_{11}^2 - T_{12}^2)^{1/2}} + \frac{[1+(-1)^{u+v}]\cos u\beta \cos v\alpha}{(T_{11}^2 - T_{22}^2)^{1/2}} + \frac{[(-1)^u + (-1)^v]\cos u\alpha \cos v\beta}{(T_{31}^2 - T_{32}^2)^{1/2}} + \frac{[(-1)^u + (-1)^v]\cos u\beta \cos v\alpha}{(T_{31}^2 - T_{42}^2)^{1/2}} \right) , \quad \text{(C7)}$$

where

$$T_{11} \equiv 1+\mu+\nu-\cos\alpha\cos\beta ,$$

$$T_{12} \equiv \mu\cos\alpha+\nu\cos\beta ,$$

$$T_{22} \equiv \mu\cos\beta+\nu\cos\alpha ,$$

$$T_{31} \equiv 1+\mu+\nu+\cos\alpha\cos\beta ,$$

$$T_{32} \equiv \mu\cos\alpha-\nu\cos\beta ,$$

$$T_{42} \equiv \mu\cos\beta-\nu\cos\alpha .$$

A numerical evaluation of (C7) using the Gaussian quadrature scheme described earlier apparently yields ten-place accuracy.

The Green's functions that involve *even* values of $w$ are given to comparable accuracy by the same stratagem, but those involving *odd* values of $w$ are given to only three or four figures. The difficulty is apparently concerned with the peculiar behavior of the auxiliary condition of (C5) over the range of integration. The accuracy of the computation may be improved (to six figures) by careful handling of the difficult regions, but a much easier procedure is to change an integral involving an odd value of $w$ to one involving an even value of $w$ by transforming the coordinates. Thus,

TABLE IV. Green's functions for the generalized fcc lattice.

| $\mu\downarrow$ $\nu\rightarrow$ | 0.25 | 0.50 | 0.75 | 1.00 | 1.33··· | 2.00 | 4.00 |
|---|---|---|---|---|---|---|---|
| 0.25 | 1.143 292 51 | 1.378 513 93 | 1.367 238 81 | 1.366 417 53 | 1.373 099 16 | 1.396 987 79 | 1.478 820 97 |
| 0.50 | | 1.359 119 45 | 1.352 521 52 | 1.352 635 03 | 1.358 400 41 | 1.378 513 93 | 1.450 424 24 |
| 0.75 | | | 1.346 823 99 | 1.346 346 29 | 1.350 443 93 | 1.366 610 62 | 1.429 309 99 |
| 1.00 | | | | 1.344 661 18 | 1.346 823 99 | 1.359 119 45 | 1.413 292 51 |
| 1.33··· | | $F^{\mu}_{\nu}(0,0,0)=F^{\nu}_{\mu}(0,0,0)$ | | | 1.346 346 29 | 1.353 767 93 | 1.397 552 14 |
| 2.00 | | | | | | 1.352 635 03 | 1.378 513 93 |
| 4.00 | | | | | | | 1.366 417 53 |
| | | | | $F(1,1,0)$ | | | |
| 0.25 | 0.461 263 19 | 0.415 962 42 | 0.390 415 47 | 0.374 059 66 | 0.359 722 94 | 0.343 382 99 | 0.325 554 15 |
| 0.50 | | 0.389 521 66 | 0.372 658 73 | 0.361 036 34 | 0.350 275 48 | 0.337 314 43 | 0.322 305 26 |
| 0.75 | | | 0.360 481 51 | 0.351 671 18 | 0.343 191 66 | 0.332 544 58 | 0.319 613 29 |
| 1.00 | | | | 0.344 661 18 | 0.337 718 97 | 0.328 717 24 | 0.317 351 14 |
| 1.33··· | | $F^{\mu}_{\nu}(1,1,0)=F^{\nu}_{\mu}(1,1,0)$ | | | 0.332 146 60 | 0.324 680 81 | 0.314 851 81 |
| 2.00 | | | | | | 0.319 029 79 | 0.311 118 94 |
| 4.00 | | | | | | | 0.305 280 41 |
| | | | | $F(1,0,1)$ | | | |
| 0.25 | 0.317 351 14 | 0.311 118 94 | 0.307 508 57 | 0.305 280 41 | 0.303 506 59 | 0.301 977 76 | 0.302 086 87 |
| 0.50 | 0.337 314 43 | 0.328 717 24 | 0.323 012 91 | 0.319 029 79 | 0.315 361 97 | 0.311 118 94 | 0.307 152 00 |
| 0.75 | 0.356 246 66 | 0.345 344 31 | 0.337 718 97 | 0.332 146 60 | 0.326 763 00 | 0.320 038 33 | 0.312 253 57 |
| 1.00 | 0.374 059 66 | 0.361 036 34 | 0.351 671 18 | 0.344 661 18 | 0.337 718 97 | 0.328 717 24 | 0.317 351 14 |
| 1.33··· | 0.396 179 93 | 0.380 633 52 | 0.369 203 64 | 0.360 481 51 | 0.351 671 18 | 0.339 908 94 | 0.324 099 55 |
| 2.00 | 0.435 666 45 | 0.415 962 42 | 0.401 108 63 | 0.389 521 66 | 0.377 550 82 | 0.361 036 34 | 0.337 314 43 |
| 4.00 | 0.528 183 59 | 0.500 363 02 | 0.478 682 24 | 0.461 263 19 | 0.442 711 42 | 0.415 962 42 | 0.374 059 66 |
| | | | | $F(0,1,1)$ | | | |
| | | | | $F^{\mu}_{\nu}(0,1,1)=F^{\nu}_{\mu}(1,0,1)$ | | | |
| | | | | $F(2,0,0)$ | | | |
| 0.25 | 0.295 319 83 | 0.258 861 60 | 0.238 153 23 | 0.224 698 09 | 0.212 648 17 | 0.198 348 02 | 0.180 983 53 |
| 0.50 | 0.273 353 36 | 0.250 230 21 | 0.235 062 28 | 0.224 302 28 | 0.214 002 44 | 0.200 894 59 | 0.183 552 35 |
| 0.75 | 0.267 028 39 | 0.248 848 86 | 0.235 986 30 | 0.226 389 74 | 0.216 824 20 | 0.204 097 53 | 0.186 271 25 |
| 1.00 | 0.267 410 30 | 0.251 114 05 | 0.239 129 05 | 0.229 936 05 | 0.220 555 27 | 0.207 731 98 | 0.189 093 54 |
| 1.33··· | 0.272 820 16 | 0.257 084 24 | 0.245 238 38 | 0.235 986 30 | 0.226 389 74 | 0.213 064 04 | 0.192 963 31 |
| 2.00 | 0.290 260 86 | 0.273 353 36 | 0.260 441 17 | 0.250 230 21 | 0.239 508 32 | 0.224 302 28 | 0.200 894 59 |
| 4.00 | 0.349 545 63 | 0.326 903 92 | 0.309 362 70 | 0.295 319 83 | 0.280 393 11 | 0.258 861 60 | 0.224 698 09 |
| | | | | $F(0,2,0)$ | | | |
| | | | | $F^{\mu}_{\nu}(0,2,0)=F^{\nu}_{\mu}(2,0,0)$ | | | |
| | | | | $F(0,0,2)$ | | | |
| 0.25 | 0.189 093 54 | 0.200 894 59 | 0.212 887 46 | 0.224 698 09 | 0.239 932 63 | 0.268 376 85 | 0.339 630 21 |
| 0.50 | | 0.207 731 38 | 0.215 761 07 | 0.224 302 28 | 0.235 934 99 | 0.258 861 60 | 0.320 077 66 |
| 0.75 | | | 0.220 555 27 | 0.226 389 74 | 0.235 009 27 | 0.253 270 16 | 0.305 874 28 |
| 1.00 | | | | 0.229 936 05 | 0.235 986 30 | 0.250 230 21 | 0.295 319 83 |
| 1.33··· | | $F^{\mu}_{\nu}(0,0,2)=F^{\nu}_{\mu}(0,0,2)$ | | | 0.239 129 05 | 0.248 784 82 | 0.285 174 43 |
| 2.00 | | | | | | 0.251 114 05 | 0.273 353 36 |
| 4.00 | | | | | | | 0.267 410 30 |
| | | | | $F(2,1,1)$ | | | |
| 0.25 | 0.218 792 60 | 0.204 393 68 | 0.195 513 40 | 0.189 476 08 | 0.183 905 34 | 0.177 131 00 | 0.168 804 91 |
| 0.50 | 0.215 675 06 | 0.204 323 17 | 0.196 675 47 | 0.191 175 09 | 0.185 870 78 | 0.179 104 44 | 0.170 264 71 |
| 0.75 | 0.215 430 61 | 0.205 518 24 | 0.198 486 42 | 0.193 243 94 | 0.188 034 95 | 0.181 159 85 | 0.171 756 21 |
| 1.00 | 0.216 422 30 | 0.207 287 39 | 0.200 586 86 | 0.195 466 71 | 0.190 269 14 | 0.183 232 35 | 0.173 255 31 |
| 1.33··· | 0.218 576 11 | 0.210 014 59 | 0.203 544 97 | 0.198 486 42 | 0.193 243 94 | 0.185 962 79 | 0.175 241 37 |
| 2.00 | 0.223 704 40 | 0.215 675 06 | 0.209 385 72 | 0.204 323 17 | 0.198 931 45 | 0.191 175 09 | 0.179 104 44 |
| 4.00 | 0.237 484 68 | 0.230 051 81 | 0.223 932 07 | 0.218 792 60 | 0.213 085 42 | 0.204 393 68 | 0.189 476 08 |
| | | | | $F(1,2,1)$ | | | |
| | | | | $F^{\mu}_{\nu}(1,2,1)=F^{\nu}_{\mu}(2,1,1)$ | | | |

TABLE IV. (*Continued*).

| $\mu \downarrow$ $\nu \rightarrow$ | 0.25 | 0.50 | 0.75 | 1.00 | 1.33··· | 2.00 | 4.00 |
|---|---|---|---|---|---|---|---|
| | | | | $F(1,1,2)$ | | | |
| 0.25 | 0.173 255 31 | 0.179 104 44 | 0.184 526 38 | 0.189 476 08 | 0.195 401 16 | 0.205 361 66 | 0.225 794 06 |
| 0.50 | | 0.183 232 35 | 0.187 301 08 | 0.191 175 09 | 0.195 978 72 | 0.204 393 68 | 0.222 715 02 |
| 0.75 | | | 0.190 269 14 | 0.193 243 94 | 0.197 086 03 | 0.204 130 46 | 0.220 456 21 |
| 1.00 | | | | 0.195 466 71 | 0.198 486 42 | 0.204 323 17 | 0.218 792 60 |
| 1.33··· | | $F^{\mu}_{\nu}(1,1,2) = F^{\nu}_{\mu}(1,1,2)$ | | | 0.200 586 86 | 0.205 032 94 | 0.217 247 26 |
| 2.00 | | | | | | 0.207 287 39 | 0.215 675 06 |
| 4.00 | | | | | | | 0.216 422 30 |
| | | | | $F(2,2,0)$ | | | |
| 0.25 | 0.227 503 23 | 0.203 360 00 | 0.190 614 59 | 0.182 837 78 | 0.176 306 36 | 0.169 254 79 | 0.162 224 40 |
| 0.50 | | 0.190 512 61 | 0.182 679 46 | 0.177 466 22 | 0.172 793 20 | 0.167 397 21 | 0.161 576 94 |
| 0.75 | | | 0.177 402 39 | 0.173 678 31 | 0.170 178 17 | 0.165 920 26 | 0.161 018 85 |
| 1.00 | | | | 0.170 889 34 | 0.168 171 73 | 0.164 725 14 | 0.160 534 62 |
| 1.33··· | | $F^{\mu}_{\nu}(2,2,0) = F^{\nu}_{\mu}(2,2,0)$ | | | 0.166 143 70 | 0.163 455 84 | 0.159 983 34 |
| 2.00 | | | | | | 0.161 664 82 | 0.159 127 98 |
| 4.00 | | | | | | | 0.157 709 18 |
| | | | | $F(2,0,2)$ | | | |
| 0.25 | 0.160 534 62 | 0.159 127 98 | 0.158 263 19 | 0.157 709 18 | 0.157 253 49 | 0.156 836 90 | 0.156 769 51 |
| 0.50 | 0.167 397 21 | 0.164 725 14 | 0.162 928 86 | 0.161 664 82 | 0.160 493 91 | 0.159 127 98 | 0.157 798 24 |
| 0.75 | 0.175 010 64 | 0.170 970 86 | 0.168 171 73 | 0.166 143 70 | 0.164 201 65 | 0.161 805 32 | 0.159 076 67 |
| 1.00 | 0.182 837 78 | 0.177 466 22 | 0.173 678 31 | 0.170 889 34 | 0.168 171 73 | 0.164 725 14 | 0.160 534 62 |
| 1.33··· | 0.193 246 91 | 0.186 209 77 | 0.181 167 77 | 0.177 402 39 | 0.173 678 31 | 0.168 847 82 | 0.162 678 06 |
| 2.00 | 0.213 338 10 | 0.203 360 00 | 0.196 062 23 | 0.190 512 61 | 0.184 920 61 | 0.177 466 22 | 0.167 397 21 |
| 4.00 | 0.266 262 96 | 0.249 733 81 | 0.237 257 03 | 0.227 503 23 | 0.217 394 13 | 0.203 360 00 | 0.182 837 78 |
| | | | | $F(0,2,2)$ | | | |
| | | | | $F^{\mu}_{\nu}(0,2,2) = F^{\nu}_{\mu}(2,0,2)$ | | | |

$$F(2,1,1) \rightarrow F(1,1,2) \quad \text{with } \mu \rightarrow \mu/\nu, \quad \nu \rightarrow 1/\nu \,. \tag{C8}$$

The values listed in Table IV were obtained by using such transformations.

The Green's functions for the generalized fcc lattice for positions through the fourth neighbor shell are given in Table IV. Each part of the table (49 integrals) required about 40 sec of computation on the IBM360-75 computer.

*Based on work performed under the auspices of the U. S. Atomic Energy Commission.

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