Random Walks in Polytype Structures*

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It is shown that the total number of walks starting and ending at the same point and having the same number of steps, is the same for all polytype structures in the fcc, hcp series and in the zincblende, wurtzite series and is independent of the starting point. This result is proved by showing that the eigenvalues of a simple Hamiltonian are the same within the two series considered. A relation is found between random walks in the two series of structures that is useful in extending currently available tables of random walks for the zincblende structure.

I. INTRODUCTION

The study of random walks on lattices is of interest in itself and plays an important role in the statistical mechanics of solids.† Many problems concerned with the thermodynamics of crystals involve the summation of diagrams on lattices which can often be related to the diagrams in a simple random walk process (e.g., the study of the Ising model above the transition temperature‡). This paper is concerned with random walks on two of the simplest series of polytype structures. The simplest structures occur in the fcc, hcp series, where the close packed layers are arranged, ABCABC... in fcc, and ABABAB... in hcp. An infinite number of other possibilities may be imagined - some with a repeating pattern and some without. All these possible structures belong to the fcc, hcp polytype series. A general discussion of polytype structures is given by Verma and Krishna‡. Polytypism may be defined, in general, as the ability of a substance to crystallize in a number of different modifications, in all of which two dimensions of the unit cell are the same while the third is a variable integral multiple of a common unit. The different polytypic modifications can be regarded as built up of layers of structure stacked parallel to each other at constant intervals along the variable dimension. The two unit-cell dimensions parallel to these layers are the same for all modifications. The third dimension depends on the stacking sequence, but is always an integral multiple of the layer spacing. Different manners of stacking these layers may result in structures having not only different morphologies but even different lattice types and space groups.‡ As well as the fcc, hcp polytype series, we also discuss the zincblende, wurtzite polytype series in this paper. Each structure in this series may be derived by placing two atoms at each site in the fcc, hcp series to form two interpenetrating sublattices. Zincblende itself has zinc on one sublattice and sulphur on the other whilst diamond is an example of a crystal having only one type of atom and the zincblende structure.

We write down a simple Hamiltonian, containing a single state at each site, that permits hopping between nearest neighbors only. The $l$th moment of the density of states formed from the eigenvalues of this Hamiltonian is just the number of ways of returning to a starting point from a walk of $l$ steps. The theorem is proved by using a unitary transformation that shows that the density of states is identical for all structures within a polytype series. It is also shown that the number of returns is independent of the starting point.

In Sec. VI, a connection is found between the density of states for the fcc, hcp series and the zincblende, wurtzite series. That such a connection exists is not surprising as each structure in the latter series may be derived from a structure in the former series. An integral expression for the density of states of the fcc and zincblende structures is used to derive a relation between the number of returns to a starting point for the two polytype series. Tables are given for the total number of returns for walks with up to nine steps in the fcc, hcp series and up to 18 steps in the zincblende, wurtzite series.

II. THE HAMILTONIAN

We define a Hamiltonian

$$H = V \sum_{(ij)} |\phi_i\rangle \langle \phi_j|,$$

where $V$ is the overlap between states $|\phi_i\rangle$ and $|\phi_j\rangle$ on
neighboring sites, the summation in (1) being restricted so that nearest neighbor pairs are counted only once. The states are normalized so that

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}.$$  

All the structures considered in this paper may be regarded as having $M$ planes stacked vertically, each plane containing $N$ atoms. The density of states $n(E)$ per atom for the Hamiltonian (1) is given by

$$n(E) = \frac{1}{(N M)} \text{Im} \sum_i \langle \phi_i | (1/E - H) | \phi_i \rangle,$$  

where the energy $E$ has a small positive imaginary part. The $l^\text{th}$ moment of the density of states is

$$\int_{-\infty}^{\infty} E^n n(E) dE = \frac{1}{(N M)} \sum_i \langle \phi_i | H^l | \phi_i \rangle = V l \gamma_l,$$  

where $\gamma_l$ is the number of returns to a given starting point in a walk of $l$ steps; an average being taken over all possible starting points in the structure and the thermodynamic limit $N, M \to \infty$ taken to eliminate surface effects. In fact it is unnecessary to take an average in (3) as it is shown at the end of Sec. IV, that $\langle \phi_i | H^l | \phi_i \rangle$ is independent of $i$ for all structures considered in this paper. For the moment, however, we are content with an average. From (3) we see that it is a necessary and sufficient condition that the density of states $n(E)$ be independent of the stacking sequence for the $\gamma_l$ also to be independent of the stacking sequence and therefore identical for all the members of the polytype series.

### III. THE FCC, HCP POLYTYPE SERIES

This series consists of close packed layers, as shown in Fig. 1, stacked vertically in the $z$ direction one on top of the other. There are three types of layers—$A, B, C$ all equivalent to within a horizontal displacement. The fcc sequence of layers is $ABCABC \cdots$ and hcp is $ABABAB \cdots$. Each close packed layer is a Bravais lattice and so it is useful to use Bloch's theorem to define states within each plane

$$|k, n\rangle = (1/\sqrt{N}) \sum_i e^{i k \cdot a} |\phi_{i,n}\rangle,$$  

where $k$ is a two-dimensional vector parallel to the plane. We use an additional label $n$ for each plane where $1 \leq n \leq M$ and the summation over $i$ is only over the $N$ states $|\phi_{i,n}\rangle$ within the plane labeled by $n$. The origin of coordinates is chosen arbitrarily for the first plane and in a manner to be prescribed for subsequent planes. We see from (1) and (4) that

$$\langle k, n | H | k, n \rangle = V \sum_{\delta} e^{i k \cdot \delta}$$

$$= 2V (\cos k_x a + 2 \cos \frac{1}{2} k_x a \cos \frac{1}{2} \sqrt{3} k_y a)$$

$$= \alpha_k$$  

where the summation over $\delta$ is over the six nearest neighbors within the plane. It is important to note that $\alpha_k$ is real and that $H$ only connects states with the same $k$ vector in accordance with Bloch's theorem. ($k$ is defined to be within the first Brillouin zone to give exactly $N$ states for each plane; the possibility of two states differing by a reciprocal lattice vector is therefore discounted.)

We now place the next layer on top of the first layer. Each atom in the first layer has three nearest neighbors in the second. We choose the atom in the second plane that lies nearest to the origin in the first plane and is in the $yz$ plane (see Fig. 1) as the origin for the second plane. This is a unique prescription and we obtain the following matrix elements between adjacent planes:

$$\langle k, n | H | k, n + 1 \rangle = \theta_k$$  

for cyclic sequence $AB, BC, CA$,

$$= \theta_k^*$$  

for anticyclic sequence $BA, CB, AC$,

where $\theta_k = V(1 + 2 \cos \frac{1}{2} k_x a \exp i \frac{1}{2} \sqrt{3} k_y a).$

Because of the translation group perpendicular to the $z$ axis, the Hamiltonian only connects states with the same $k$ vector in adjacent planes. From Eqs. (5) and (6), we see that by using Bloch's theorem perpendicular to the $z$ axis, the Hamiltonian is split into $N$ blocks each one being $M \times M$ and characterised by a $k$ vector. We can consider the eigenvalues of each block separately. For hcp we have an $ABABAB \cdots$ stacking sequence and the structure of one of the blocks is

$$\begin{bmatrix}
\alpha & \theta & \theta^* & \alpha & \theta \\
\theta & \alpha & \theta & \theta & \theta \\
\theta^* & \alpha & \theta & \theta & \theta^* \\
\theta & \theta & \theta & \theta & \theta \\
\theta & \theta & \theta & \theta & \theta \\
\end{bmatrix},$$

where the $k$ label on $\alpha, \theta$ has been dropped and the only nonzero elements lie on and just above and below the diagonal. The layers are stacked alternatively cyclically, AB and anticyclically, BA and so we get a sequence $\theta \theta^* \theta \theta^* \theta$ above the diagonal. The

*FIG. 1.* The three possible stacking positions for the fcc, hcp series. The $x, y$ axes lie in the plane perpendicular to the stacking axis $z$. The distance between nearest neighbors in the plane is $a$ and the distance between successive layers is $c = \sqrt{3} a$. A polytype structure may be constructed from any sequence of the three layers $A, B,$ and $C$ provided only that the same layer does not occur twice in adjacent layers, e.g., $ABCBACBC$ is allowed whereas $BBBBBA$ is not.

eigenvalues of (8) are unaltered by any unitary transformation. The row and column indicated by arrows in (6) are multiplied by $\hat{\theta}$ and $\hat{\theta}^*$, respectively. The transformed matrix becomes

\[
\begin{pmatrix}
\alpha & \theta & \theta^* & \theta \\
\theta & \alpha & \theta & \theta^* \\
\theta^* & \alpha & \theta & \theta \\
\theta & \theta^* & \alpha & \theta \\
\end{pmatrix}
\]

and the stacking sequence that leads to (9) is $ABACAB\cdots$, i.e., the second $B$ has been changed to $C$. It is clear, therefore, that we can have either $B$ or $C$ between two $A$'s, $A$ or $B$ between two $C$'s, or $C$ or $A$ between two $B$'s, and the Hamiltonian (1) will have the same eigenvalues. A little thought will convince the reader that any desired sequence may be generated by this procedure. For example, we can go from hcp to fcc in the following way:

\[
\begin{align*}
A & \quad B & \quad A & \quad B & \quad A & \quad B & \quad A & \cdots \\
A & \quad B & \quad C & \quad B & \quad A & \quad B & \quad A & \cdots \\
A & \quad B & \quad C & \quad A & \quad C & \quad B & \quad A & \cdots \\
A & \quad B & \quad C & \quad A & \quad C & \quad A & \quad B & \cdots \\
A & \quad B & \quad C & \quad A & \quad B & \quad A & \quad C & \cdots \\
A & \quad B & \quad C & \quad A & \quad B & \quad A & \quad C & \cdots \\
\end{align*}
\]

(10)

It is clear that we are generating an fcc sequence. We are also generating a CBA for every ABC, and will therefore finish up with a structure half of which is $ABCACAB\cdots$ and the other half $CABACAB\cdots$. There will be an interface between these two sequences; however it will have negligible weight in the thermodynamic limit. We could generate hcp from fcc by reversing the above procedure used in (10).

If we count a cyclic sequence $AB, BC, CA$ as $+1$ and an anticyclic sequence $BA, CB, AC$ as $-1$, then the sum of all these numbers for a given structure may be called the cyclicity $C$ of that structure and is conserved under the unitary transformation described in this section. Thus the hcp structure with an odd number of layers has $C = 0$, whereas the fcc structure has $C = M - 1$, where $M$ is the number of layers. A structure with cyclicity $-C$ can be formed from a structure with cyclicity $+C$ by reflection in the xy plane. Therefore by inserting an appropriate small number of interfaces (one in the case of hcp to fcc), it is possible to generate any structure and the interfaces will have negligible weight in the thermodynamic limit.

The equivalence of the number of returns in a random walk on the fcc and hcp lattices was first demonstrated by C. Domb and M. F. Sykes. Their approach involves the detailed consideration of lattice diagrams and it is not easy to see how it would generalize to all close packed structures.

### IV. The Zincblende, Wurtzite Polytype Series

The zincblende, wurtzite series is rather more complex than the fcc, hcp series and contains two kinds of atoms that may be called $a$ and $b$. We define each atom in the fcc, hcp series to be of type $a$. A structure in the zincblende, wurtzite series can be formed from one in the fcc, hcp series by placing an atom of type $b$ a distance $\frac{1}{2}c$ above each $a$ type atom in the $x$ direction (see Fig. 1). The structure now consists of two identical interpenetrating sublattices with each atom in one sublattice having four nearest neighbors in the other sublattice at the corners of a tetrahedron. We may visualize this structure as consisting of puckered planes, stacked vertically, and containing $a$ type atoms from the $(n+1)$th layer with $b$ type atoms from the nth layer a distance $\frac{1}{2}c$ below and displaced horizontally so that the nearest neighbor bonds form hexagonal chains. Each atom has three nearest neighbors in this puckered plane and each $a$ type atom has a nearest neighbor $b$ in the plane above. The translational symmetry of the structure perpendicular to the $z$ axis can again be used to define a two-dimensional $k$ vector. We now have two kinds of states for the $n$th layer, $k, n, a$ for sublattice $a$ and $k, n, b$ for sublattice $b$. We thus have

\[
\langle k, n, a | H | k, n, b \rangle = V
\]

(11)

for the vertical bonds and

\[
\langle k, n, b | H | k, n + 1, a \rangle = \delta_k \text{ for cyclic sequence } AB, BC, CA,
\]

\[
= \delta_k \text{ for anticyclic sequence } BA, CB, AC,
\]

(12)

where $\delta_k$ is defined in (7) and the origin of coordinates in each $a$ type layer is chosen in the way described in the previous section. If we start with the wurtzite structure which is derived from hcp and therefore stacked $ABABAB\cdots$, each of the $N$ blocks of $H$ characterized by a two-dimensional $k$ vector looks like

\[
\begin{pmatrix}
0 & V \\
V & 0 \\
\theta^* & 0 & V \\
\theta & 0 & \theta^* \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
0 & V \\
V & 0 \\
\theta^* & 0 & V \\
\theta & 0 & \theta^* \\
\end{pmatrix}
\]

(13)

where we have suppressed the $k$ label on $\theta$ and the basis states for the matrix are ordered $|k, n, a\rangle, |k, n, b\rangle, |k, n + 1, a\rangle, |k, n + 1, b\rangle\cdots$. We perform
the unitary transformation in which the two rows indicated are multiplied by \( \theta / \theta' \) and the two columns are multiplied by \( \theta' / \theta \). The sequence above the diagonal becomes \( V_0 V_0' V_0 V_0' V_0 V_0' \) which corresponds to \( ABA \rightarrow ABA \ldots \). This is the same change in sequencing that we achieved for the fcc, hcp series in the previous section and the argument, therefore, proceeds in an identical manner from this point to show that the density of states is the same for any desired sequence.

As a footnote to the preceding two sections, it can be seen that the diagonal elements of \( H_1 \) are equal within each of the \( M \) blocks in the Hamiltonian in either of the two polytype series, provided that end effects are neglected of course. This is because in the diagonal elements of \( H_1 \), a given \( \theta \) is always multiplied by its conjugate \( \theta' \). Therefore \( \langle \phi_i | H | \phi_i \rangle \) is independent of \( i \) and so the random walk can begin at any site and the number of returns will be the same. This important result allows us to remove the \( (1/NM) \sum_i \) in Eq. (5). Any site is "typical" in respect to random walks as long as it is sufficiently far from the surface that the walk does not reach the surface. This result is perhaps a little surprising as all the structures considered in this paper, except fcc, contain sites not related by a vector in the translation group of the structure.

V. DISCUSSION

It is amusing to notice that the two structures considered in Secs. III and IV, which have the interesting property with respect to random walks, are the closest packed (12 neighbors) and loosest packed (4 neighbors) of the three-dimensional structures. The main interest is in the equivalence of the random walks; however, the equivalence of the density of states for the Hamiltonian (1) is also of some interest.

We have found it convenient in this work not to define a wave vector \( k_z \) in the direction of the random stacking. To do so is misleading even in the case of structures periodic in the \( z \) direction as the essential simplicity is obscured. As an illustration of this we consider the fcc and hcp structures in the 001 direction. Defining a wave vector \( k_z \), the dispersion \( E_{001} \) along 001 for the hcp, where the separation between adjacent planes is \( c = (\sqrt{2} / 3) a \), is given by the eigenvalues of a \( 2 \times 2 \) matrix,

\[
\begin{bmatrix}
6V & 3V(1 + e^{i2k_z c}) \\
3V(1 + e^{i2k_z c}) & 6V
\end{bmatrix},
\]

i.e., \( E_{001} = 6V(1 + \cos k_z c) \)

These two branches are shown in Fig. 2. The Brillouin zone has a hexagonal cross section perpendicular to the \( k_z \) axis and a height \( 2\pi / 2c \) in the \( k_z \) direction. It is possible to describe the fcc lattice in a similar manner although it is more usual to exploit the cubic symmetry to its greatest extent and have only one atom in each unit cell, so that \( z \) axis becomes a 111 direction. However, we can define a \( k_z \) vector and the dispersion \( E_{001} \) along 001 is now given by the eigenvalues of a \( 3 \times 3 \) matrix,

\[
\begin{bmatrix}
6V & 3V & 3V e^{3i k_z c} \\
3V & 6V & 3V \\
3V e^{-3i k_z c} & 3V & 6V
\end{bmatrix},
\]

i.e., \( E_{001} = 6V(1 + \cos k_z c + \pi / 3) \).

These three branches are also shown in Fig. 2. The Brillouin zone again has a hexagonal cross section perpendicular to the \( k_z \) direction but its height is only \( 2\pi / 3c \) corresponding to a repeat distance of \( 3c \) for the fcc structure as opposed to \( 2c \) for hcp. This zone is only \( 1 / 3 \) the size of the Brillouin zone that is usually used for the fcc structure; however, every \( k \) vector has three modes associated with it instead of just one. It can be seen immediately from Fig. 2 that the energies are the same for the two cases as required by the result of Sec. 3; however, the \( k \) space description is quite different; in particular the zero energy mode is at the zone center in hcp and at the zone boundary in fcc. As the period in the \( z \) direction gets longer, the height of the Brillouin zone shrinks and the number of modes associated with each \( k \) vector increases until in the limit of no periodicity in the \( z \) direction, \( k_z \) becomes zero and there are \( M \) modes associated with each \( k \) vector in the plane perpendicular to the \( z \) axis.

In the theory of magnetic insulators, the Heisenberg Hamiltonian with nearest neighbor ferromagnetic coupling is often used. Within the states of one-spin deviation, this Hamiltonian reduces to the simple hopping Hamiltonian (1) apart from a constant. Thus the density of spin waves states is the same for all structures in the fcc, hcp series and in the zincblende, wurtzite series.

It is probable that the work of this paper can be extended to more complex Hamiltonians than Eq. (1) provided that the hopping is restricted to nearest neighbors only. Recently, Thorpe and Wearie have shown that the density of states for a model of Si or Ge containing four states per atom (when spin is not considered) in a tetrahedrally coordinated structure can be related to the density of states of the Hamiltonian (1) by a structure independent transformation. Thus for this model the density of states for Si and Ge in the valence and conduction bands is independent of the structure within the zincblende, wurtzite polytype

![FIG. 2. The dispersion relation along the (001) direction for the hcp and fcc structures. The Brillouin zone is hexagonal in cross section perpendicular to the \( z \) axis and has a repeat distance of \( 2\pi / 2c \) for hcp and \( 2\pi / 3c \) for fcc along the \( z \) direction. This corresponds to the conventional zone for hcp, but the zone for fcc is \( 1 / 3 \) of the conventional zone for that structure. The figure illustrates that the eigenvalues are the same for the two lattices even though the labeling of the states in \( k \) space is quite different.](image)
series. This leads to the import result that the band gap is also structure independent. The problem of the difference in the band structure for the zincblende and wurtzite structures when the hopping is not restricted to nearest neighbors and when two atomic species are present, has been considered by Birman.\(^4\)

VI. RELATION BETWEEN THE TWO SERIES

In this section we derive a simple relationship between the number of returns \(r_1\) in random walks on the two polytype series considered in this paper. It is convenient to fix our attention upon the simplest member of each series, i.e., fcc and zincblende. It is not surprising that the \(r_1\) for these two lattices are related as zincblende is the fcc lattice with two atoms at each lattice point.

The fcc lattice has one atom in the unit cell and this has 12 nearest neighbors which we may put at \((\pm 1, \pm 1, 0), a(0, \pm 1, 0), a(0, 0, \pm 1)\). The eigenvalues \(E_{k}^{(i)}\) of the Hamiltonian (1) are given by

\[
E_{k}^{(i)} = \frac{1}{V} \sum_{\delta} e^{i k \cdot \delta} = \frac{4}{V} V_{i x y z}
\]

where

\[
\alpha_{x y z} = \cos k_x a \cos k_y a + \cos k_y a \cos k_z a + \cos k_z a \cos k_z a. \tag{19}\]

The wave vector \(k\) is of course three-dimensional and the sum over \(\delta\) is over the 12 nearest neighbors. Via (3), the \(r_1\) for the fcc lattice (denoted by \(r_{1}^{(f c c)}\)) are given by

\[
r_{1}^{(f c c)} = \frac{1}{V^{2} N M} \sum_{k} \left( E_{k}^{(f c c)} \right)^{l}
= 4! \frac{1}{(2\pi)^{3}} \int_{-\pi}^{\pi} \int_{n}^{n} (1 + \cos x \cos y + \cos y \cos z + \cos z \cos x)^{l} dx dy dz. \tag{20}\]

The integrals in (20) can easily be evaluated for small values of \(l\) using

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} \cos 2nx dx = \frac{(2\pi)!}{4^{l}(n!)^{2}},
\]

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} \cos 2n + 1 x dx = 0
\]

where \(n\) is an integer. The \(r_{1}^{(f c c)}\) for 1 up to 9 are given in Table I. They agree with the values given by Domb\(^1\) for the fcc and hcp lattices.

The zincblende structure has two atoms at each lattice point of an fcc lattice. Each atom on one sublattice has four nearest neighbors on the other sublattice with may put at \(a/2(1, 1, 1), a/2(1, -1, -1), a/2(-1, -1, 1)\) and \(a/2(-1, 1, -1)\). The eigenvalues \(E_{k}^{(b)}\) for the zincblende structure are obtained from the \(2 \times 2\) matrix

\[
\begin{bmatrix}
0 \\
V_{k}^{b} e^{i(k_{x} + k_{y}) a} + e^{i(k_{x} - k_{y}) a} + e^{i(k_{y} + k_{z}) a} + e^{i(k_{x} + k_{z}) a} + e^{i(k_{y} + k_{z}) a} + e^{i(k_{x} + k_{y}) a}
\end{bmatrix}
\]

where \(\alpha_{x y z}\) also occurs in the dispersion relation for the fcc lattice and is given by (19). The number of

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TABLE I. The number of returns to the origin \(r_1\) for the first few walks on the fcc, hcp polytype series [calculated from Eq. (20)] and for the zincblende, wurtzite polytype series [calculated from Eq. (24)].

returns \(r_{1}^{(b)}\) for the zincblende are obtained from (3) and (22):

\[
r_{1}^{(b)} = \frac{1}{V^{2} N M} \sum_{k} \left( E_{k}^{(b)} \right)^{l}
= 4! \frac{1}{(2\pi)^{3}} \int_{-\pi}^{\pi} \int_{n}^{n} (1 + \cos x \cos y + \cos y \cos z + \cos z \cos x)^{l} dx dy dz, \tag{23}\]

where \(l\) is an integer. There are no returns involving walks with an odd number of steps. The summation over \(k\) is over both branches of the spectrum (22).

It is clear that from (20) and (23) we can derive a simple relation between \(r_{1}^{(f c c)}\) and \(r_{1}^{(b)}\)

\[
r_{1}^{(b)} = \sum_{m=0}^{l} 4^{m-1} \left( \frac{1}{l} \right) r_{1}^{(f c c)}. \tag{24}\]

We have used (24) to derive \(r_{1}^{(b)}\) for \(l\) up to 18. This extends the table given by Domb\(^1\) for the diamond structure which goes to \(l = 12\). The results are shown in Table I. Notice that there are no returns consisting of an odd number of steps. This is because all the members of the zincblende, wurtzite series can be split into two interpenetrating sublattices as described in Sec. IV.

The density of states for the Hamiltonian (1) for the fcc lattice has been calculated numerically by Frikke\(^8\) and expressed in terms of elliptic integrals by Joyce.\(^8\) Using (18) and (22), the density of states for the zincblende structure can be found by a simple transformation on the density of states for the fcc lattice.\(^6\)

VII. CONCLUSIONS

We have shown that the density of states for a simple hopping Hamiltonian is the same for all structures in the fcc, hcp polytype series and in the zincblende, wurtzite polytype series. This result is then used to show that the number of returns to the origin in a walk starting from any point and having a given number of steps is the same for all members of each of the two polytype series. A relationship is given between random walks on the two sets of structures.

Note added in proof: I would like to thank M. E. Fisher for informing me of his unpublished proof of the equivalence of random walks on the lattices of the fcc, hcp polytype structures. This rather elegant proof utilizes generating functions (see Ref. 1) and its extension to the zincblende, wurtzite polytype series is discussed briefly in the Appendix of J. F. Nagle, J. Math. Phys. 7, 1484 (1968).

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1 C. Domb, Advan. Phys. 9, 245 (1960).
5 See, for example, C. Kittel, Quantum Theory of Solids (Wiley, New York, 1963), Chap. 4.