where

$$g_l(k, r, r') = (i/2k)(-1)^l [w_l(kr) w_l(-kr') - w_l(-kr) w_l(kr')] .$$

Now just as in the one-dimensional case C_l *is treated as a parameter*. Using the relationship between $u_l(z)$ and $w_l(\pm z)$ and the linearity of (18), we get [in analogy to (4)]

$$\varphi_l(r) = i(-1)^{l+1} f_l(-k, r)(C_l + \tfrac{1}{2}A_l) + i(\tfrac{1}{2}A_l) f_l(k, r) , \tag{19}$$

with

$$f_l(k, r) = w_l(kr) - \int_r^\infty dr' g_l(k, r, r') V(r') f_l(k, r') \tag{20}$$

[Compare with Eq. (3.8), Ref. 4]. Note that this equation is easily iterated in the same way as (5). Now combine (17) and (19) to find

$$C_l = \tfrac{1}{2}A_l [f_l(k)/f_l(-k) - 1] = \tfrac{1}{2}A_l [S_l(k) - 1], \tag{21}$$

where the Jost function $f_l(k)$ is given by

$$f_l(k) = 1 + (1/k) \int_0^\infty dr f_l(k, r) V(r) u_l(kr) \tag{22}$$

and $S_l(k)$ is the S-matrix element for $V(r)$ [see Eqs. (4.4) and (4.5) of Ref. 4]. We finally obtain (see again Ref. 4)

$$\varphi_l(r) = kr\psi_l(r) = i(\tfrac{1}{2}A_l) \frac{1}{f_l(-k)} [f_l(-k) f_l(k, r) - (-1)^l f_l(-k, r) f_l(k)] . \tag{23}$$

This analysis has shown the intimate connection between the techniques developed in Ref. 1 and the "Jost-function method" as used in scattering theory. It is possible that the detailed knowledge, already developed,[4–6] of the Jost functions (especially $l = 0$) can be applied toward an understanding of the random-potential problem in one dimension. Further comment is inappropriate for a paper of this sort.

ACKNOWLEDGMENT

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[1] J. F. Reading and J. L. Sigel, Phys. Rev. B 5, 556 (1972).

[2] Regarding the work of Ref. 1, I remark that it can easily be extended to the study of the effect of localized impurities, added to a periodic potential in one dimension, on the states of an isolated band. This follows since the unperturbed Green's function for such a band has a form to which the methods of Ref. 1 can be applied. This point will be discussed in greater detail in a later publication.

[3] This discussion is intimately connected to some work, now in preparation, of J. L. Sigel and J. F. Reading on the solution of the wave equation in three dimensions for a particle moving among a set of very-short-range potentials of arbitrary strength and position. The method presented here represents a generalization of that work to a continuous potential which, however, must be spherically symmetric.

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[5] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[6] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

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Band Structure of a Tight-Binding Hamiltonian

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Thorpe and Weaire have discovered a simple relationship between the density of states of a model Hamiltonian for a tetrahedrally bonded amorphous solid and the density of states of a much simpler Hamiltonian. Here is given a simple derivation of that result. . The case of a compound semiconductor is also discussed.

I. INTRODUCTION

Weaire[1] has proposed a certain tight-binding Hamiltonian[2] to discuss a tetrahedrally bonded solid which is "topologically disordered"—that is, a solid for which every bond and site interaction is the same, and for which every site has exactly four neighbors bonded to it, but which lacks long-range order in the network structure.

Thorpe and Weaire[3] recently showed that there is a simple relationship between the density of states of this Hamiltonian and that of a much simpler one. Their derivation involved the resummation of the diagrams of the Green's-function perturbation theory. It will be shown here how their result can be derived from the properties of the operators that appear in the Weaire Hamiltonian.

II. DEFINITIONS

At each site i of the network there are four orbital states[4] $|\phi_{ij}\rangle$ $(j=1, \ldots, 4)$. It is assumed that every state of the system can be expressed as a linear combination of the ϕ_{ij}. Let us now define the operator

$$\hat{A}_i = \tfrac{1}{4} \sum_{j,j'} |\phi_{ij}\rangle\langle\phi_{ij'}| \ , \tag{1}$$

which is an interaction of the bonds common to the site i;

$$\hat{A} = \textstyle\sum_i \hat{A}_i \tag{2}$$

and

$$\hat{T} = \sum |\phi_{ij}\rangle\langle\phi_{i'j}| \ , \tag{3}$$

where the sum ranges over all nearest-neighbor pairs ii', and $|\phi_{ij}\rangle$ $(|\phi_{i'j}\rangle)$ is the bond on $i(i')$ which points towards $i'(i)$. The operator $\hat{T}$ interchanges the coefficients of these orbitals. The operators $\hat{A}_i$ are normalized so that they are all projections, and the only eigenfunction with nonvanishing eigenvalue is

$$|i\rangle = \tfrac{1}{2}\textstyle\sum_j |\phi_{ij}\rangle \ . \tag{4}$$

The operator $\hat{A}$ is also a projection; it discards the part of any function which is linearly independent of the $|i\rangle$. The operator $\hat{T}$ also has an interesting property: It is its own inverse:

$$\hat{T}^2 = \hat{I} \tag{5}$$

because to interchange twice is to have no effect. In terms of these operators, Weaire's Hamiltonian is

$$\hat{H} = 4\, V_1 \hat{A} + V_2 \hat{T} \tag{6}$$

apart from an additive term $-V_1$ which will be ignored throughout what follows. In the physically relevant cases V_1 and V_2 are negative.

III. SIMPLIFICATION OF HAMILTONIAN

From the definition of H and the properties of A and T it follows that

$$\hat{H}^2 - 4\, V_1 \hat{H}\hat{A} - 4 V_1 \hat{A}\hat{H} = V_2^2 \hat{I} - 16\, V_1^2 \hat{A} \ . \tag{7}$$

The right-hand side commutes with $\hat{A}$, and consequently, the left-hand side and $\hat{A}$ can be simultaneously diagonalized. Let us restrict our attention to the subspace of eigenfunctions of $\hat{A}$ with unit eigenvalue: Multiply the above equation by $\hat{A}$ from the right-hand side. Further, substitute for the rightmost $\hat{H}$ from its definition and get

$$(\hat{H}^2 - 4 V_1 \hat{H})\hat{A} - 4 V_1 V_2 \hat{A}\hat{T}\hat{A} = V_2^2 \hat{A} \ . \tag{8}$$

The term $\hat{A}\hat{T}\hat{A}$ commutes with $\hat{A}$ and thus can be diagonalized within the proper subspace of $\hat{A}$; let the eigenfunction with eigenvalue $\frac{1}{4}\epsilon$ be Φ_ϵ;

$$\hat{A}\hat{T}\hat{A}\ \Phi_\epsilon = \tfrac{1}{4}\epsilon\, \Phi_\epsilon, \quad \hat{A}\Phi_\epsilon = \Phi_\epsilon \ . \tag{9}$$

Then we have found the spectrum of the operator $\hat{H}^2 - 4 V_1 \hat{H}$:

$$(\hat{H}^2 - 4 V_1 \hat{H})\, \Phi_\epsilon = (V_1 V_2 \epsilon + V_2^2)\, \Phi_\epsilon \ . \tag{10}$$

The spectrum E of $\hat{H}$ itself is related to that of $(\hat{H}^2 - 4 V_1 \hat{H})$ in the obvious way so that we may write

$$E^2 - 4 V_1 E = V_1 V_2 \epsilon + V_2^2 \ , \tag{11}$$

which is equivalent to the first line of Eq. (17) of Ref. 3.

The operator $\hat{A}\hat{T}\hat{A}$, which Thorpe and Weaire call the "one-band Hamiltonian," is a much simpler operator than H itself; it can be written in terms of the orbitals $|i\rangle$ as

$$\hat{A}\hat{T}\hat{A} = \frac{1}{4} \sum_{i,i'} |i\rangle\langle i| \ , \tag{12}$$

where the sum ranges over all nearest-neighbor pairs i and i'. Thus we need consider only one function per site.

The functions Φ_ϵ are not eigenfunctions of $\hat{H}$, but the eigenfunctions Ψ of $\hat{H}$ can be constructed from them; explicitly they are $\Psi = (2V_1 + Q + V_2\hat{T})\Phi_\epsilon$ with eigenvalue $E = 2V_1 + Q$ and $\Psi = (2V_1 - Q + V_2\hat{T})\Phi_\epsilon$ with eigenvalue $E = 2V_1 - Q$, where $Q = (4V_1^2 + V_2^2 + V_1 V_2 \epsilon)^{1/2}$.

The remaining structure of the spectrum of $\hat{H}$ (according to Thorpe and Weaire) is a pair of δ functions at $E = \pm V_2$. The existence of a large number of localized states (associated with closed rings of sites) having these eigenvalues can be demonstrated[3]; the corresponding wave functions all lie within the null space of $\hat{A}$. This feature seems to depend on more specific properties of the Hamiltonian than just $\hat{A}^2 = \hat{A}$ and $\hat{T}^2 = \hat{I}$.

IV. COMPOUND SEMICONDUCTORS

Let us imagine that the network can be broken into two sets X and Y of sites, such that the p neighbors of each X site are all Y sites, and the q neighbors of each Y site are all X sites. Let $\hat{X}$ be the projection operator which separates out all orbitals on the X sites, and similarly for $\hat{Y}$. We can then define a model semiconducting compound with the Hamiltonian

$$H = a\hat{A}\hat{X} + b\hat{A}\hat{Y} + x\hat{X} + y\hat{Y} + t\hat{T} \ , \tag{13}$$

where a, b, x, y, and t are arbitrary real coefficients. Thorpe and Weaire[3] propose a special case of this with $a = b = 4V_1$, $x = V_0 = -y$, and $t = V_2$.

In addition to the properties of the various operators already noted, we can add that $\hat{A}$ commutes with $\hat{X}$ and $\hat{Y}$, and that the only matrix elements of $\hat{T}$ are between the two sets of sites, so that $\hat{X}\hat{T}\hat{X} = \hat{Y}\hat{T}\hat{Y} = 0$ and $\hat{X}\hat{T} = \hat{T}\hat{Y}$.

Let us assume we know a solution to the "one-band" problem encountered above, and note that

$$\hat{X}\hat{A}\hat{T}\hat{A}\hat{T}\Phi_\epsilon = \hat{A}\hat{T}\hat{A}\hat{T}\hat{X}\Phi_\epsilon = \tfrac{1}{16}\epsilon^2 \hat{X}\Phi_\epsilon \ , \tag{14}$$

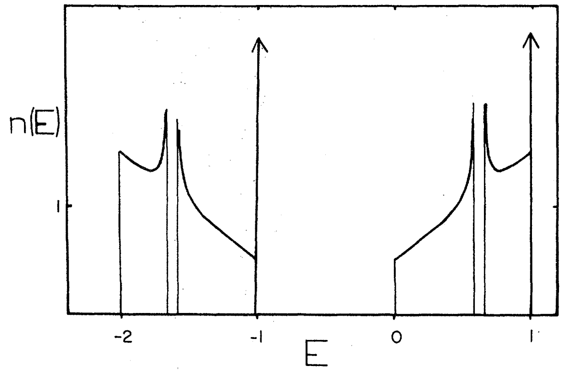

FIG. 1. Density of states for the compound semiconductor. It was assumed that the one-band Hamiltonian has a flat density of states in the range $-4<\epsilon<4$; the parameters of Eq. (16) were chosen to be $x=0.1=-y$, $a=b=t=-1$.

so that $\phi = \hat{X}\Phi_\epsilon$ is a function defined just on the X sublattice which is an eigenfunction of $\hat{A}$ with eigenvalue 1 and of $\hat{A}\hat{T}\hat{A}\hat{T}$ with eigenvalue $\frac{1}{16}\epsilon^2$. Now with good reason we can suspect that there are eigenfunctions of $\hat{H}$ of the form

$$\psi=\phi+\alpha\hat{T}\phi+\beta\hat{A}\hat{T}\phi+\gamma\hat{T}\hat{A}\hat{T}\phi\ , \tag{15}$$

and in fact, construction of the equation $\hat{H}\psi=E\psi$ and equating the coefficients of ϕ, $\hat{T}\phi$, $\hat{A}\hat{T}\phi$, and $\hat{T}\hat{A}\hat{T}\phi$ shows that E is a solution of

$$[(E-x)(E-y-b)-c^2][(E-y)(E-x-a)-c^2] = \tfrac{1}{16}\, abc^2\,\epsilon^2 \tag{16}$$

and

$$\begin{aligned} \alpha &= c(E-x)\ , \\ \beta &= a(E-y)\,\alpha/[(E-y)(E-x-a)-c^2]\ , \\ \gamma &= [c/(E-y)]\beta\ . \end{aligned} \tag{17}$$

Since (16) is a quartic equation, there are four solutions for E, so that, in general, there will be four bands. Figure 1 shows a typical case, in which it was assumed that ϵ ranges from -4 to $+4$ with a flat density of states.[5] The square-root singularity at the band edge will occur whenever the density of states of the one-band Hamiltonian is constant near $\epsilon=0$ (as occurs for the Bethe lattice, but not the diamond cubic structure[3]). Also shown are the δ functions which presumably occur for E such that

$$(E-x)(E-y)=c^2\ . \tag{18}$$

Weaire and Thorpe inform me that they have achieved similar results by another method.

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[1] D. L. Weaire, Phys. Rev. Letters 26, 1541 (1971); D. L. Weaire and M. F. Thorpe, Phys. Rev. B 4, 2508 (1971).

[2] G. Leman and J. Friedel, J. Appl. Phys. 33, 281 (1962).

[3] M. F. Thorpe and D. L. Weaire, Phys. Rev. B 4, 3518 (1971).

[4] The result does not depend on the coordination number; four is chosen here because it is the physically relevant choice.

[5] The case shown corresponds to the top strip of Fig. 3 of Ref. 3.

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Comment on the Tight-Binding Model for Amorphous Semiconductors

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A new proof is given for the existence of a band gap in the Heine-Thorpe-Weaire model of an amorphous semiconductor.

In a recent series of articles, Heine, Weaire, and Thorpe[1-3] (HWT) have examined the properties of a simple tight-binding model for amorphous semiconductors. The model is specified by assuming that there are four equivalent orbitals associated with each site and that these orbitals form bonds with each of the nearest neighbors. The spatial arrangement of the atoms is disordered, but it is assumed that each atom still has four nearest neighbors. The one-electron Hamiltonian is then

$$H=\sum_{\substack{n\\ i\neq j}}|ni\rangle\, V_1\langle nj| + \sum_{n,i}|ni\rangle\, V_2\langle n_i'i| \equiv H_1+H_2\ . \tag{1}$$