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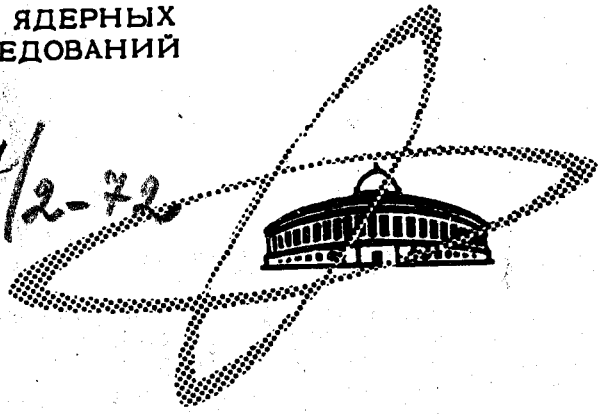

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THE ELECTRONIC DENSITY OF STATES IN THE WEAIRE MODEL OF AN AMORPHOUS SOLID

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THE ELECTRONIC DENSITY OF STATES IN THE WEAIRE MODEL OF AN AMORPHOUS SOLID

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Using a simple tight-binding model, it is possible to show the existence of a band gap in a tetrahedrally bonded solid of arbitrary structure[1]. Recently Thorpe and Weaire[2] have studied this model in detail. They have found an expression for the density of states which relates it to a one band Hamiltonian and involves the influence of structure and overlap parameters in a well separated form. Thorpe and Weaire obtain this result, using a diagrammatic expansion for the Green function, in a relatively complicated way. In the following a compact and much simpler derivation for the density of state formula of Thorpe and Weaire is given.

With a suitable choice of the energy zero the model Hamiltonian[2] may be written as

$$H = \sum_{n \neq n',\, i} |in\rangle V_2 \langle n'i| + \sum_{n,\, i,\, j} |in\rangle V_1 \langle nj| \,, \qquad (1)$$

where the atoms are labelled by n , n' and the bonds by i , j . The first term in (1)

$$H_0 = \sum_{n \neq n',\, i} |in\rangle V_2 \langle n'i| \qquad (2)$$

describes the overlap along the same bonds between neighbouring atoms with eigenvalues $E = \pm V_2$ per bond. The other term in (1)

$$W = \sum_{n,i,j} | in \rangle V_1 \langle nj | \qquad (3)$$

involves the overlap between orbitals associated with the same atom. W describes decoupled atoms, each with a non-degenerate eigenstate $| sn \rangle$ at energy $E = 4 V_1$ and three degenerate eigenstates at $E = 0$. These eigenstates are nothing but the atomic eigenstates with angular momentum $L = 0, 1$. Therefore W is in the main a projection operator

$$W = 4 V_1 P \quad , \quad P = \sum_n | sn \rangle \langle ns | \quad , \qquad (4)$$

which projects out the s-part of the wave function.

It is simpler to consider the integrated density of states than the density of states. The integrated density of states per atom $N(E)$ may be expressed as

$$N(E) = N_0(E) - \frac{1}{\pi N} Im. \, Tr \ell n (1 - W G_0(E)) \qquad (5)$$

with

$$N_0(E) = \frac{1}{\pi N} Im \; Tr \ell n G_0(E) \qquad (6)$$

the integrated density of states of the Hamiltonian H_0 and with

$$G_0(z) = (z - H_0)^{-1} \tag{7}$$

the appropriate Green operator. Using the projection operator P (4) and the properties of the trace for the second term in (5) we obtain

$$Tr\ell n\,(1 - W\,G_0\,(E)) = Tr\ell n(1 - 4\,V_1\,P\,G_0(E)P)\,. \tag{8}$$

An elementary calculation gives

$$P\,G_0(E)\,P = \frac{1}{E^2 - V_2^2}\,(E\,P + \frac{1}{4}\,V_2 \sum_{n \neq n'} |\,s\,n\rangle\langle n'\,s\,|)\,. \tag{9}$$

With (9) and the definition

$$\zeta = E^2 - V_2^2 - 4\,V_1\,E\,, \tag{10}$$

$$h = \sum_{n \neq n'} |\,s\,n\rangle\langle n'\,s \tag{11}$$

the integrated density of states may be written as

$$N(E) = \frac{1}{2}\,N_0(E) - \frac{1}{\pi N}\,Im\;Tr\ell n(\zeta - V_1\,V_2\,h)\,. \tag{12}$$

Only the second term depends on the topological order. This term describes the density of states of a one band Hamiltonian h (11) with an overlap parameter $V_1\,V_2$.

With the eigenvalues ϵ_ν of h we obtain for the integrated density of states

$$N(E) = \theta(E - V_2) + \theta(E + V_2) - \frac{1}{\pi N} \sum_\nu Im \ln(\zeta - V_1 V_2 \epsilon_\nu) \quad (13)$$

and thus for the density of states $D(E)$ the result first derived by Thorpe and Weaire

$$D(E) = \delta(E - V_2) + \delta(E + V_2) - \frac{1}{\pi N} \sum_\nu Im \frac{\frac{d\zeta}{dE}}{\zeta - V_1 V_2 \epsilon_\nu} . \quad (14)$$

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