

## Effects of short-range order on the spectral density function for a one-dimensional amorphous solid\*

D. G. Hall<sup>†</sup>

*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37916  
and Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830*

J. S. Faulkner

*Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830*

(Received 1 July 1976)

The spectral density  $A(Q, E)$  is calculated exactly for a one-dimensional model of an amorphous solid. The model contains an adjustable short-range order parameter  $\alpha$ , and  $A(Q, E)$  is calculated for several values of  $\alpha$ . The harmonic-oscillator Hamiltonian appropriate to lattice vibrations and a tight-binding Hamiltonian describing in a simplified way either electrons or spin waves are studied for nearest-neighbor interactions. The calculated spectral densities are compared with the recent neutron-scattering measurements of Mook, Wakabayashi, and Pan.

### I. INTRODUCTION

The study of elementary excitations in disordered systems has received considerable attention in the last several years. Applications<sup>1-3</sup> of the coherent-potential approximation (CPA) of Soven<sup>4</sup> have shown that the CPA provides an acceptable level of understanding of the properties of excitations in substitutionally disordered binary alloys. In structurally disordered systems such as liquid metals and amorphous solids, the necessity to include the effects of short-range correlations in the atomic positions introduces added complexity. While there have been several attempts to obtain a CPA-level theory which adequately treats short-range order, none has achieved complete success. Peterson, Schwartz, and Butler (PSB)<sup>5</sup> have recently compared exact calculations of the electronic integrated density of states for a one-dimensional liquid metal to the results of three approximate theories. They found that neither the non-self-consistent quasicrystalline approximation of Lax<sup>6</sup> nor the self-consistent approximations of Schwartz and Ehrenreich,<sup>7</sup> and Gyorffy<sup>8</sup> (as extended by Korringa and Mills<sup>9</sup>) agreed with the exact results in the strong-scattering regime. A recent analysis by Olson<sup>10</sup> has shown that the Anderson-McMillan<sup>11</sup> prescription is also unsatisfactory. Other attempts such as the effective medium approximation of Roth<sup>12</sup> have not been thoroughly tested and appear quite complicated to apply to even a simple model.

In essentially all of this work attention has been focused on calculating either the density of states or the integrated density of states.<sup>13</sup> In this paper, we present a numerical investigation of the effects of short-range order on the spectral density function  $A(Q, E)$  for excitations in a structurally dis-

ordered solid. The spectral density is calculated exactly for one-dimensional models described by harmonic-oscillator and tight-binding Hamiltonians. The method of calculation, the model, and the Hamiltonians considered will be discussed in detail in Sec. II. In Sec. III, the results of the calculation will be presented. Section IV provides a brief discussion of the experimental implications of these calculations which will serve to explain some of the motivation for this study. A summary and discussion of other possible applications of our methods and results appear in Sec. V.

### II. NUMERICAL ASPECTS

The spectral density  $A(\vec{Q}, E)$  is defined by

$$A(\vec{Q}, E) = -(1/\pi) \text{Im}G(\vec{Q}, E), \quad (1)$$

where  $G(\vec{Q}, E)$  is the Fourier transform in space and time of the single-particle Green's function. For constant  $E$ , the ordered-system spectral density consists of  $\delta$  functions situated at the values  $Q(E)$  obtained from the appropriate dispersion relation. In calculating the spectral density for a disordered system, one seeks the configuration averaged quantity  $\langle A(\vec{Q}, E) \rangle$  where  $\langle \dots \rangle$  denotes an average over all possible configurations in the statistical ensemble. In what follows, the averaging brackets will be omitted and  $A(\vec{Q}, E)$  will refer to the configuration-averaged quantity unless otherwise noted.

The statistical model chosen for this study is based upon the so-called "hard-rod" distribution function for the classical one-dimensional fluid.<sup>14</sup> This model has been used recently in the work of PSB<sup>5</sup> mentioned above.  $N$  line segments of length  $a$  are distributed on a line of length  $Nl$ , the only condition on the distribution being that they cannot

overlap. The atomic positions in the hard-rod model are the centers of these line segments. If  $\alpha = a/l$  is equal to one, the system is periodic with lattice constant  $l$ , while the totally random or Poisson distribution of atoms corresponds to  $\alpha = 0$ . Any intermediate degree of disorder can be obtained by a suitable choice of  $\alpha$ . The probability of finding a nearest-neighbor atom at a distance  $x$  from a given atom is

$$p(x) = [\theta(x-a)/(l-a)] e^{(x-a)/(l-a)}, \quad (2)$$

where  $\theta(x-a)$  is one for  $x > a$  and zero for  $x < a$ . In what follows, the parameter  $l$  is set equal to unity.

The calculation of the spectral density  $A(Q, E)$  is very much the same for both the tight-binding system and the vibrational system. We describe the details for the former below, and point out the differences occurring for the latter thereafter. The tight-binding Hamiltonian is given by

$$H\psi(n) = K_n\psi(n) + M_n\psi(n-1) + M_{n+1}\psi(n+1), \quad (3)$$

and is appropriate for a simplified description of electrons or spin waves. In Eq. (3),  $\psi(n)$  gives the probability amplitude for finding an excitation at site  $n$ ,  $K_n$  and  $M_n$  are the diagonal and off-diagonal matrix elements, respectively. In modeling the system, we set  $K_n = 1$  for all  $n$  and choose for  $M_{n+1}$  an exponential dependence upon the equilibrium spacing  $d_{n+1} = (x_{n+1} - x_n)$  between sites  $n+1$  and  $n$ ,

$$M_{n+1} = M_0 \exp(1 - d_{n+1}/l). \quad (4)$$

By choosing  $M_0 = -\frac{1}{2}$ , the ordered system ( $\alpha = 1$ ) dispersion relation becomes

$$E(Q) = 2\sin^2(\frac{1}{2}Q). \quad (5)$$

The spectral density for this Hamiltonian takes the form

$$A(Q, E) = \lim_{N \rightarrow \infty} \frac{1}{N} \left\langle \sum_j |\exp(-iQx_n)\psi_j(x_n)|^2 \delta(E - E_j) \right\rangle, \quad (6)$$

where  $\psi_j$  and  $E_j$  are the  $j$ th eigenfunction and eigenvalue of the Hamiltonian, and  $x_n$  is the equilibrium position of site  $n$ . To calculate  $A(Q, E)$  we follow the formalism developed by Halperin.<sup>15</sup> Let us introduce the functions  $y(n; E)$  and  $\phi(n; E)$  such that

$$y(n; E) = M_n \phi(n-1; E) / \phi(n; E). \quad (7)$$

The function  $\phi(n; E)$  is defined for each configuration in the ensemble and each energy  $E$  to be the unique solution of the equation

$$(K_n - E)\phi(n; E) + M_n\phi(n-1; E) + M_{n+1}\phi(n+1; E) = 0, \quad (8)$$

subject to the conditions

$$y(1; E) = y_0, \quad (9)$$

and

$$y(N+1; E) = y_N, \quad (10)$$

where  $y_0$  and  $y_N$  are arbitrary constants. Upon defining the function

$$U_1(n; E) = \sum_{n'=1}^{n-1} \exp(-iQx_{n'}) \times \phi(n'; E) / \exp(-iQx_n) \phi(n; E), \quad (11)$$

Eq. (6) can be written in the simplified form

$$A(Q, E) = \lim_{N \rightarrow \infty} (1/N) \langle |U_1(N+1; E)|^2 \times \delta(y_N - y(N+1; E)) \rangle. \quad (12)$$

The  $\delta$  function in Eq. (12) requires that the value of  $E$  for which  $|U_1(N+1; E)|^2$  is evaluated be an eigenvalue. As the eigenvalues will be very closely spaced in energy and since  $A(Q, E)$  cannot depend upon the particular value of  $y_N$  chosen, we evaluate  $A(Q, E)$  by averaging over a set of values of  $y_N$  and Eq. (12) becomes

$$A(Q, E) = \lim_{N \rightarrow \infty} (1/N) \langle |U_1(N+1; E)|^2 \rangle. \quad (13)$$

The convergence properties of  $A(Q, E)$  as calculated from Eq. (13) are rather different from those encountered in calculating a quantity such as the integrated density of states  $n(E)$ . In a Monte Carlo calculation of  $n(E)$  for electronic excitations in a one-dimensional disordered system, for example,  $n(E)$  can be related to the number of nodes per unit length of the wave function.<sup>16</sup> The number of nodes per unit length is an ergodic quantity and convergence can be obtained by using a sufficiently long chain of atoms. In calculating  $A(Q, E)$  from Eq. (13), however, increasing the number of atoms in a given chain does not, in general, increase the precision in determining  $A(Q, E)$ . It can be shown<sup>17</sup> that the mean  $M\{\dots\}$  and variance  $V\{\dots\}$  of the random variable  $A^c(Q, E) = (1/N)|U_1(N+1; E)|^2$  are given by

$$\lim_{N \rightarrow \infty} M\{A^c(Q, E)\} = A(Q, E), \quad (14)$$

and

$$\lim_{N \rightarrow \infty} V\{A^c(Q, E)\} \neq 0, \quad (15)$$

in general. That is, even for an infinite system ( $N \rightarrow \infty$ ) the quantity  $A^c(Q, E)$  is, for each  $Q$  and  $E$ , a random variable with unknown distribution function and mean value  $A(Q, E)$ . As an example, if the stochastic process  $\phi(n; E)$  were normally distributed, then  $A^c(Q, E)$  would be exponentially distributed with mean value  $A(Q, E)$  and variance

$A^2(Q, E)$ .<sup>18</sup> The variance can be made to approach zero for large  $N$  by calculating, instead of  $A(Q, E)$ , the average of  $A(Q, E)$  over a finite range of  $Q$ . However, the limit  $N \rightarrow \infty$  remains difficult to achieve since the amplitude of the wave function increases exponentially with  $N$ .<sup>19</sup> To further reduce the variance, we have calculated our averaged  $A(Q, E)$  for 100 statistically independent chains (with  $N = 500$ ) and performed a second average. Increasing either  $N$  or the number of chains does not appreciably affect the results.

The procedure for calculating the vibrational system spectral density  $A(Q, \omega)$  parallels the one just described. The Hamiltonian is given by

$$H = \sum_n \frac{p_n^2}{2m} + \sum_n \beta_{n+1} (U_{n+1} - U_n)^2, \quad (16)$$

where  $p_n$  and  $U_n$  are the momentum and displacement operators for the atom of mass  $m$  (set to unity) at site  $n$ . The spring constant  $\beta_{n+1}$  couples the atoms at sites  $n$  and  $n+1$ , and is assumed to depend upon  $d_{n+1}$  according to

$$\beta_{n+1} = \beta_0 \exp(1 - d_{n+1}/l). \quad (17)$$

Choosing  $\beta_0 = 1$  leads to the ordered-system dispersion relation

$$\omega(Q) = 2|\sin(Q/2)|. \quad (18)$$

The spectral density  $A(Q, \omega)$  is given by

$$A(Q, \omega) = \frac{1}{N} \left\langle \sum_j \left| \sum_{n=1}^N \exp(iQx_n) U_j(n) \right|^2 \delta(\omega - \omega_j) \right\rangle, \quad (19)$$

where the displacements  $U_j(n)$  are solutions of

$$\beta_{n+1} U_j(n+1) + \beta_{n-1} U_j(n-1) - (2\beta_n - \omega_j^2) U_j(n) = 0. \quad (20)$$

Performing the same steps which lead to Eq. (13) reduces the spectral density to the form

$$A(Q, \omega) = \lim_{N \rightarrow \infty} \frac{2\omega}{N} \langle |U_1(N+1; E)|^2 \rangle, \quad (21)$$

which differs from Eq. (13) by a factor of  $2\omega$ . The convergence properties of both Eq. (13) and Eq. (21) are identical and no further discussion is needed here.

### III. RESULTS

The spectral density  $A(Q, \omega)$  for the vibrational (phonon) system described by Eq. (16) is shown in Fig. 1 for  $\alpha = 0.75$  and  $\omega = 0.50$ . The positions of the ordered-system  $\delta$  functions are obtained from Eq. (18) and are indicated by arrows in the figure. Long-wavelength excitations are rather insensitive to the absence of long-range ordered as evi-

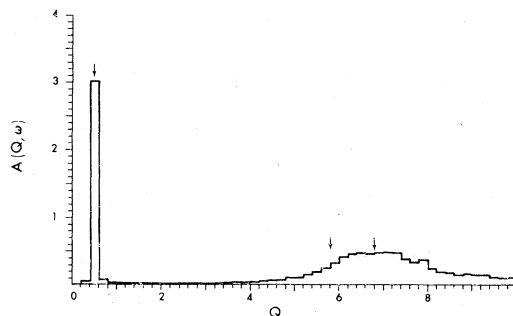


FIG. 1. Spectral density  $A(Q, \omega)$  as a function of  $Q$  for  $\omega = 0.50$  and  $\alpha = 0.75$  for the vibrational system. Arrows indicate positions of ordered-system  $\delta$  functions.

denced by the sharpness of the peak in  $A(Q, \omega)$  near  $Q = 0$ . In the "second zone"  $A(Q, \omega)$  is no longer distinguishable as two separate peaks and appears as a single broad structure shifted toward higher  $Q$  from the ordered-system positions. Plotted in Fig. 2 are the spectral densities as a function of  $Q$  for  $\alpha = 0.85$  and four values of fixed  $\omega$ . The first peak in  $A(Q, \omega)$  has been omitted for each  $\omega$  for ease of presentation. The arrows, once again, represent the positions of the ordered-system ( $\alpha = 1$ )  $\delta$  functions as will be the case in the remainder of this work. The effect of short-range order for  $\alpha = 0.85$  is to produce a broadened version of the ordered-system dispersion of the

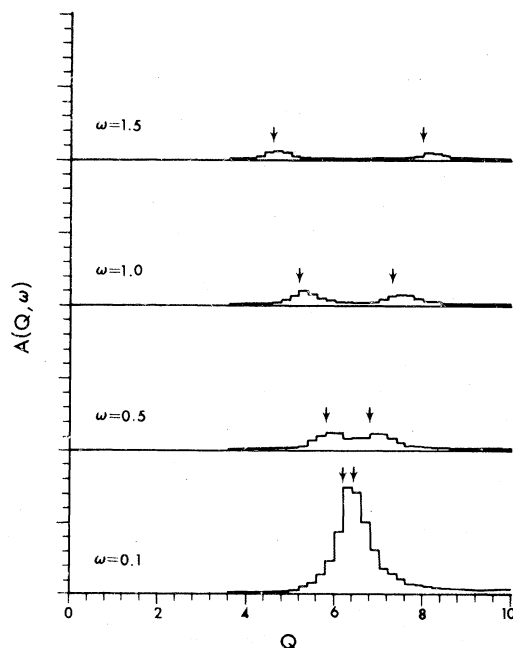


FIG. 2. Spectral density  $A(Q, \omega)$  as a function of  $Q$  for  $\alpha = 0.85$  and four values of  $\omega$  for the vibrational system. Arrows indicate positions of ordered-system  $\delta$  functions.

ordinary phonon excitations. The strong weighting of the states at small  $\omega$  can be understood by comparison with the ordered-system spectral density which is given by<sup>20</sup>

$$A(Q, \omega) = (1/2\omega)\delta(\omega - \omega(Q)) - \delta(\omega + \omega(Q)). \quad (22)$$

The spectral density for a periodic system is characterized by a weighting factor of  $\omega^{-1}$ . Unless the states move considerably in  $\omega - Q$  space when  $\alpha$  is decreased from unity to 0.85, the  $\omega^{-1}$  dependence will require that  $A(Q, \omega)$  have strong weighting for small  $\omega$ . The broadening of the peaks in  $A(Q, \omega)$  for small  $\omega$  produces a single peak in the "second zone" for  $\omega < 0.50$ . In Fig. 3 are the results of the calculation for the same four values of  $\omega$  with  $\alpha$  reduced to  $\alpha = 0.75$ . Note that the scale in Fig. 3 has been reduced by a factor of ten relative to Fig. 2. For  $\alpha = 0.75$ , the features of the spectral density are broader than those for  $\alpha = 0.85$  and are shifted even more toward higher  $Q$ .  $A(Q, \omega)$  for  $\omega = 0.10$  is no longer the most heavily weighted as was the case for  $\alpha = 0.85$ . Figures 4 and 5 point out more clearly the broadening and shifting of the structure in  $A(Q, \omega)$  with decreasing  $\alpha$  for  $\omega = 0.10$  and  $\omega = 0.50$ , respectively. In both cases, all vestiges of the ordered system peaks in the spectral density have vanished for  $\alpha = 0.50$ .

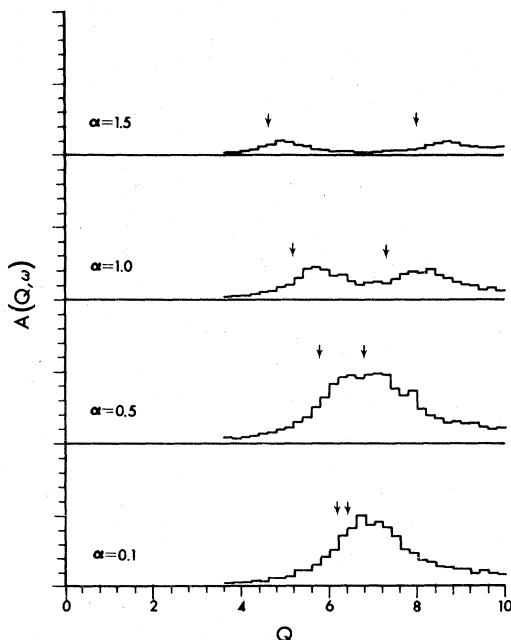


FIG. 3. Spectral density  $A(Q, \omega)$  as a function of  $Q$  for  $\alpha = 0.75$  and four values of  $\omega$  for the vibrational system. Arrows indicate positions of ordered-system  $\delta$  functions. The scale has been reduced by a factor of ten relative to Fig. 2.

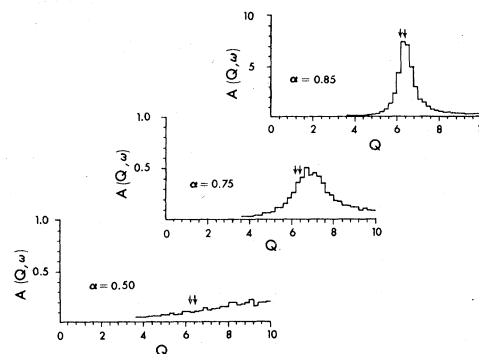


FIG. 4. Spectral density  $A(Q, \omega)$  as a function of  $Q$  for  $\omega = 0.10$  and three values of  $\alpha$  for the vibrational system. Arrows indicate positions of ordered-system  $\delta$  functions.

The features observed in the spectral density for the phonon system are very similar to those of the tight-binding system. Shown in Fig. 6 are the tight-binding system spectral densities for  $\alpha = 0.85$  and four values of fixed energy. The most striking difference between Fig. 6 and the equivalent plot for the phonon system (Fig. 2) is the difference in weighting of  $A(Q, E)$ . The  $\omega^{-1}$  dependence of the spectral density is peculiar to the phonon system and is not a feature of the tight-binding system. The plots in Fig. 6 indicate that the states at small  $E$  receive diminished weighting relative to those at larger  $E$  in the "second zone." As with the phonon system, the dominant effect of short-range order for  $\alpha = 0.85$  is to produce a broadened and slightly shifted version of the ordered system dispersion. Upon decreasing  $\alpha$  to 0.75 we obtain the spectral densities of Fig. 7. The scale of Fig. 7 has been reduced by a factor of two relative to Fig. 6. The broadening of  $A(Q, E)$  and the shifting of the peaks toward higher  $Q$  continues for  $\alpha = 0.75$ . The weighting of the states is

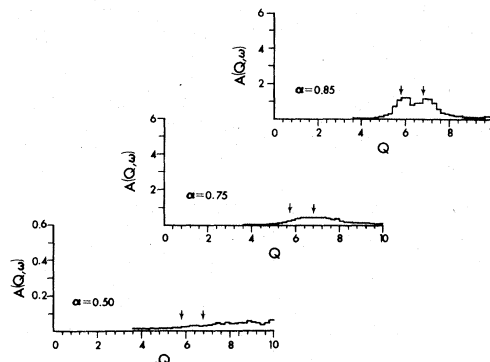


FIG. 5. Spectral density  $A(Q, \omega)$  as a function of  $Q$  for  $\omega = 0.50$  and three values of  $\alpha$  for the vibrational system. Arrows indicate positions of ordered-system  $\delta$  functions.

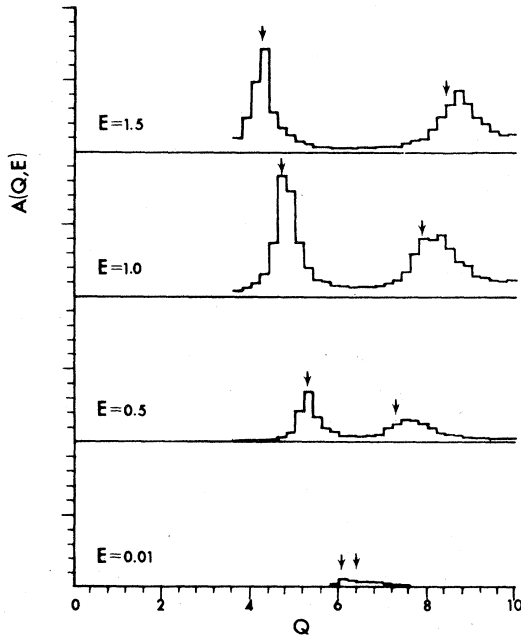


FIG. 6. Spectral density  $A(Q, E)$  as a function of  $Q$  for  $\alpha = 0.85$  and four values of  $E$  for the tight-binding system. Arrows indicate ordered-system  $\delta$  functions.

such that the mid-band energy  $E = 1.0$  becomes the strongest feature in the "second zone." In Fig. 8, we show plots of the spectral density as a function of  $Q$  for  $E = 0.50$  and several values of  $\alpha$ . As with the phonon system the sharp features of  $A(Q, E)$  gradually diminish with decreasing  $\alpha$  until at  $\alpha = 0.50$  nothing remains of the ordered-system behavior.

Recent numerical calculations of the dynamic form factor and the alloy spectral density have been given by Alben and Thorpe<sup>21</sup> and Alben *et al.*,<sup>22</sup> respectively. In their method of calculating the spectral density, one calculates  $G(\vec{Q}, E)$  by performing a space and time Fourier transform of the Green's function obtained by numerically solving the time-dependent equation of motion. The spectral density is obtained from  $G(\vec{Q}, E)$  according to Eq. (1). In addition to the method described above in the discussion leading to Eq. (13), we have calculated the spectral density for our tight-binding model using this "equation-of-motion" method with periodic boundary conditions. In calculating  $A(Q, E)$  we employed 20-, 40-, and 80-atom chains and 250 iterations of the equation of motion. The results obtained from this technique were quite similar to those presented above, although we had not yet reached convergence for the 80-atom chain.

Axe<sup>23</sup> has recently calculated the dynamic form factor  $S(Q, \omega)$  using a one-dimensional model of an amorphous solid for which an analytic solution

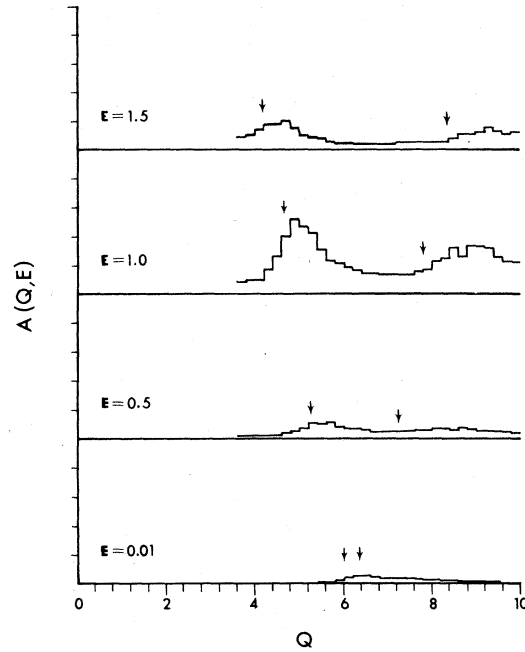


FIG. 7. Spectral density  $A(Q, E)$  as a function of  $Q$  for  $\alpha = 0.75$  and four energies. Arrows indicate positions of ordered-system  $\delta$  functions. Scale has been reduced by a factor of 2 relative to Fig. 6.

is possible. The feature of that model which makes a closed form solution possible is the neglect of force constant variations. That is, Axe's model assumes the force constants are independent of atomic separations, an assumption not made in this study.

#### IV. RELATION TO EXPERIMENT

The results of Sec. III can be used to gain insight into the very general features of excitations

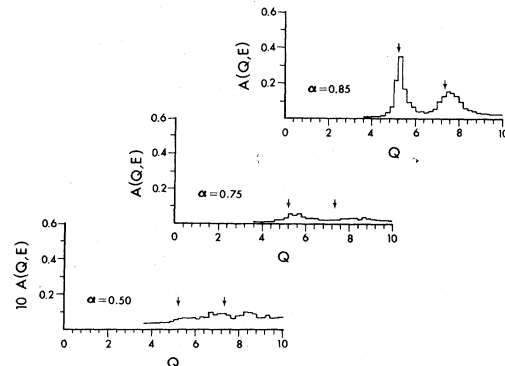


FIG. 8. Spectral density  $A(Q, E)$  as a function of  $Q$  for  $E = 0.50$  and three values of  $\alpha$ . Arrows indicate positions of ordered-system  $\delta$  functions.

in three-dimensional systems. Unlike the density of states, the spectral density contains no systematic distortions which stem from the one-dimensionality of the system. The spectral density as utilized here provides a description of the effects of structural disorder upon the one-particle states of the model system. In the theory of neutron scattering, the differential-scattering cross section can be written

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{Q_2}{2\pi Q_1} S(\vec{Q}, \omega), \quad (23)$$

where  $\vec{Q}_1$  and  $\vec{Q}_2$  are the initial and final momenta of the incident neutron,  $d\Omega$  is an infinitesimal volume element, and  $S(\vec{Q}, \omega)$  is the dynamic form factor. Expanding  $S(\vec{Q}, \omega)$  and neglecting those terms describing multiple excitations gives<sup>24</sup>

$$S(Q, \omega) = Ne^{-2W(Q)} [I(Q)\delta(\omega) + Q^2A(Q, \omega)]. \quad (24)$$

In Eq. (24),  $I(Q)$  gives the strength of the elastic scattering contribution while the spectral density  $A(Q, \omega)$  gives the strength of the inelastic scattering from single-particle excitations. The Debye-Waller factor  $2W(Q)$  diverges in one dimension and so we cannot actually calculate  $S(Q, \omega)$  or the scattering cross section. However, this is of no importance for this study as scattering from a hypothetical one-dimensional chain is unphysical. The spectral density is the quantity of importance as it describes the single-particle excitation states in the presence of structural disorder. To the extent to which our one-dimensional system can be taken as a model for the effects of short-range order in a solid, the spectral densities in Figs. 1–8 can be used to interpret the qualitative features of neutron scattering measurements.

The existence of a “second zone” in the one-particle excitation spectrum obtained from liquid-like structures is well known. Randolph and Singwi,<sup>25</sup> for example, have shown that the “phonon” dispersion curve for liquid lead is quite similar in the “second zone” to that of the solid. An approximate calculation by Hubbard and Beeby<sup>26</sup> has also produced a “phonon” dispersion curve for liquid structures resembling that for a solid. Our calculations suggest that a solidlike dispersion curve is likely to be a general feature of the one-particle excitation spectrum associated with structurally disordered systems.

Mook, Wakabayashi, and Pan<sup>27</sup> have recently reported neutron inelastic scattering studies of the amorphous ferromagnetic system  $\text{Co}_4\text{P}$ . Some results of their measurements are shown in Fig. 9, where the neutron scattering intensity is plotted as a function of  $Q$  for several energies.<sup>28</sup> At some energy  $E_1$ , one observes a small peak centered between two larger ones. With decreasing energy,

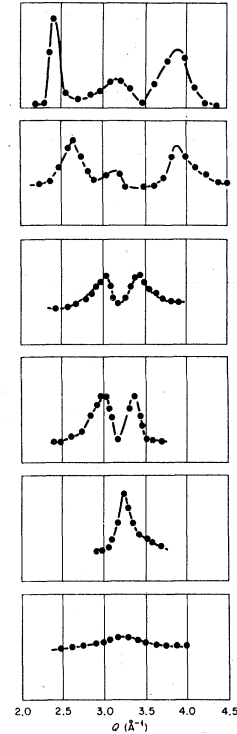


FIG. 9. Neutron-scattering intensity as a function of  $Q$  for several energies (energy increases vertically) from Mook *et al.* (Refs. 27 and 28).

the pattern becomes double-peaked and at an energy which we shall call  $E_0$ , finally becomes single-peaked. Below  $E_0$ , there exists a small broad structure independent of energy and located near the first peak in the liquid-structure factor  $S(Q)$  (near  $Q = 3.13 \text{ \AA}^{-1}$ ). In analyzing this data, Mook *et al.* suggested that if one were to neglect the small central peak at  $E_1$  and the small structures below  $E_0$ , the peak positions of the remaining features could be plotted<sup>27</sup> as shown in Fig. 10, a dispersion relation reminiscent of that observed for rotons<sup>29</sup> in liquid helium. While the curve in Fig. 10 is quite similar to the roton dispersion curve, there is also a rather striking similarity between the measurements and our calculated  $A(Q, \omega)$  for the tight-binding system.<sup>30</sup> This similarity leads one to speculate that the observations might be explained as a manifestation of the effects of structural disorder upon the ordinary spin waves of the system. This view is consistent with the recent work of Alben<sup>31</sup> who found rotonlike behavior in three-dimensional models with structural disorder. If such an interpretation is valid, the structure below  $E_0$  in Fig. 9 would correspond to structures such as that shown in Fig. 6 for  $E = 0.01$ . This interpretation, however, is not without problems. If one draws

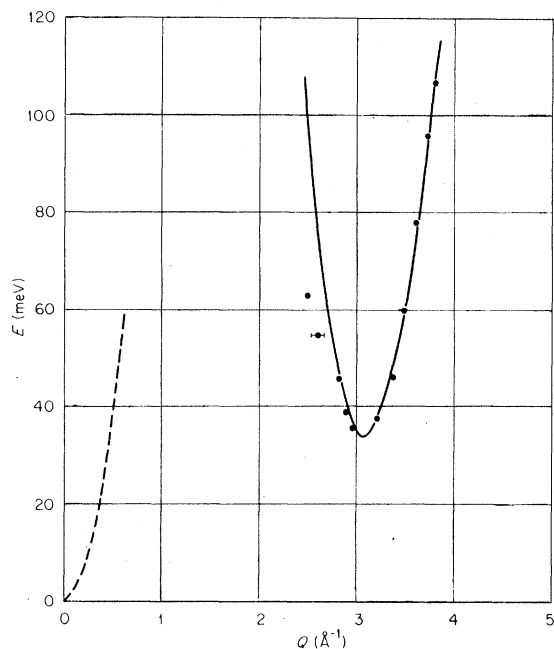


FIG. 10. Suggested analysis of data in Fig. 9; from Mook *et al.* (Ref. 27).

an analogy between the amorphous and polycrystalline states, one does not expect to observe split peaks in the second "zone."<sup>32</sup> In fact, this interpretation seems to indicate that the scattering from  $\text{Co}_4\text{P}$  is more similar to scattering from a crystal than a polycrystal. It is hoped that this calculation will stimulate further work on three-dimensional systems from which more direct inferences can be drawn.

## V. SUMMARY

We have presented a Monte Carlo calculation of the spectral density  $A(Q, E)$  for a one-dimensional model of an amorphous solid. The calculated spectral density was used to examine the effects of short-range order upon the single-particle excitations described by the harmonic oscillator and tight-binding Hamiltonians. The insight gained from the model calculations has been used to examine the recent neutron scattering measurements of Mook *et al.* The measured excitation spectrum was observed to be qualitatively similar to our tight-binding results suggesting that these excitations might be explained as the remnants of the ordinary spin-wave excitations in a system possessing short-range order.

The procedure described in Sec. II for performing a Monte Carlo calculation of the spectral density can be applied to other one-dimensional problems. One of us (D.G.H.) has compared the spectral density obtained in the quasicrystalline approximation (QCA)<sup>6</sup> to the exact result obtained by the method of Sec. II for electronic excitations in a one-dimensional liquid metal.<sup>33</sup> A comparison of the CPA and exact spectral densities for electronic excitations in a one-dimensional alloy is in progress.

## ACKNOWLEDGMENTS

The authors wish to thank Drs. J. J. Olson and W. H. Butler for thoughtful discussions during the course of this work. We also wish to thank Dr. H. A. Mook for interesting conversations regarding the measurements discussed above.

\*Research sponsored by the ERDA under contract with the Union Carbide Corp.

†Supported in part by a grant from ERDA administered by Oak Ridge Associated Universities.

<sup>1</sup>S. Kirkpatrick, B. Velický, and H. Ehrenreich, *Phys. Rev. B* **1**, 3250 (1970).

<sup>2</sup>G. M. Stocks, R. W. Williams, and J. S. Faulkner, *Phys. Rev. B* **4**, 4390 (1971).

<sup>3</sup>G. M. Stocks, R. W. Williams, and J. S. Faulkner, *J. Phys. F* **3**, 1688 (1973).

<sup>4</sup>P. Soven, *Phys. Rev.* **156**, 809 (1967).

<sup>5</sup>H. K. Peterson, L. M. Schwartz, and W. H. Butler, *Phys. Rev. B* **11**, 3678 (1975).

<sup>6</sup>M. Lax, *Rev. Mod. Phys.* **23**, 287 (1951); *Phys. Rev.* **85**, 621 (1952).

<sup>7</sup>L. M. Schwartz and H. Ehrenreich, *Ann. Phys. (N.Y.)* **64**, 100 (1971).

<sup>8</sup>B. L. Gyorffy, *Phys. Rev. B* **1**, 3290 (1970).

<sup>9</sup>J. Korrington and R. L. Mills, *Phys. Rev. B* **5**, 1654 (1972).

<sup>10</sup>J. J. Olson, *Phys. Rev. B* **12**, 2908 (1975).

<sup>11</sup>P. W. Anderson and W. L. McMillan, *Proceedings of the International School of Physics "Enrico Fermi," Course 37*, edited by W. Marshall (Academic, New York, 1967).

<sup>12</sup>L. Roth, *Phys. Rev. B* **9**, 2476 (1974).

<sup>13</sup>For a review, see P. Dean, *Rev. Mod. Phys.* **44**, 127 (1972); or R. J. Elliott, J. A. Krumhansl, and P. L. Leath, *ibid.* **46**, 465 (1974).

<sup>14</sup>Z. W. Salzburg, R. W. Zwanzig, and J. G. Kirkwood, *J. Chem. Phys.* **21**, 1098 (1953).

<sup>15</sup>B. I. Halperin, *Phys. Rev.* **139**, A104 (1965).

<sup>16</sup>H. M. James and A. S. Ginzburg, *J. Phys. Chem.* **57**, 840 (1953).

<sup>17</sup>A. A. Sveshnikov, *Applied Methods of the Theory of Random Functions* (Pergamon, London, 1966).

<sup>18</sup>E. Parzen, *Stochastic Processes* (Holden-Day, San Francisco, 1964).

<sup>19</sup>R. E. Borland, *Proc. R. Soc. Lond.* **274**, 529 (1963).

<sup>20</sup>See, for example, S. Doniach and E. Sondheimer, *Green's Functions for Solid State Physicists* (Benjamin, Reading, 1974).

- <sup>21</sup>R. Alben and M. F. Thorpe, *J. Phys. C* 8, L275 (1975).
- <sup>22</sup>R. Alben, M. Blume, H. Krakauer, and L. Schwartz, *Phys. Rev. B* 12, 4090 (1975).
- <sup>23</sup>J. D. Axe, Proceedings of the Rhode Island Summer School, 1974 (unpublished).
- <sup>24</sup>See, for example, J. Callaway, *Quantum Theory of the Solid State* (Academic, New York, 1974).
- <sup>25</sup>P. D. Randolph and K. S. Singwi, *Phys. Rev.* 152, 99 (1966).
- <sup>26</sup>J. Hubbard and J. L. Beeby, *J. Phys. C* 2, 556 (1969).
- <sup>27</sup>H. A. Mook, N. Wakabayashi, and D. Pan, *Phys. Rev. Lett.* 34, 1029 (1975).
- <sup>28</sup>This figure differs slightly from that presented in Ref. 23 and was provided by H. A. Mook (private communication).
- <sup>29</sup>D. G. Henshaw and A. D. B. Woods, *Phys. Rev.* 121, 1244 (1961).
- <sup>30</sup>A preliminary discussion of this work can be found in the Proceedings of the Conference on Neutron Scattering, Gatlinburg, Tennessee, June, 1976 (unpublished).
- <sup>31</sup>R. Alben, *AIP Conf. Proc.* 29, 136 (1976).
- <sup>32</sup>See, for example, T. E. Faber, *Theory of Liquid Metals* (Cambridge U.P., Cambridge, 1972).
- <sup>33</sup>D. G. Hall, *Solid State Commun.* 20, 509 (1976).