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Elementary excitations in disordered systems with short-range order*

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A general theory for elementary excitations in disordered systems with short-range order has been developed. The theory is based on an averaging formalism which is a generalization of an averaging technique introduced by Mookerjee. The theory is valid for excitations in all mean-free-path regions and can be used to generate analytic Green's functions which have the proper translational symmetry. The mathematical formalism is discussed for random alloys and amorphous solids. Illustrative calculations for Markov chains are shown to compare well with essentially exact numerical calculations.

I. INTRODUCTION

In earlier works,[1,2] we have described a theory for elementary excitations in randomly disordered solids which correctly treats off-diagonal as well as diagonal disorder. The theory is based on a technique for averaging functions of independent random variables which was introduced by Mookerjee.[3,4] Using this theory, we are able to generate translationally invariant Green's functions which can describe both the long- and short-mean-free-path regions of the disordered system and which are always analytic.

Since this averaging formalism is restricted to considering only functions of independent random variables it cannot be applied to disordered systems with short-range order, which includes many alloys, amorphous solids and liquids. In order to include short-range order, we must be able to average functions of dependent random variables.

In this paper, we show how the averaging formalism can be generalized so as to include functions of dependent random variables. We call this averaging technique the augmented space formalism (ASF). Using the ASF we can construct a general theory for elementary excitations in disordered systems which can include short-range order as well as off-diagonal and diagonal disorder.

Despite the general nature of this new theory, it is conceptually similar to the theory described in Ref. 2 (hereafter referred to as I). As before, rather than averaging the real-space Green's functions directly, we construct a nonrandom Hamiltonian defined on a new Hilbert space which we have called the augmented space. This new space can be described as the direct product of the Hilbert space spanned by the original Hamiltonian with a "disorder" space which describes the various allowed configurations of the disordered system. The new nonrandom Hamiltonian is defined such that configurational averages in real space are equal to inner products in the augmented space.

Once the augmented space is constructed we can evaluate the configurationally averaged Green's function by applying the recursion method of Haydock, Heine and Kelley[5] or any of a number of other techniques.[6-8] The essential step in the theory is the transformation to augmented space.

The paper is divided into six sections. In Sec. II, the formalism for averaging functions of dependent random variables is described. The application of the ASF to elementary excitations in disordered alloys with short-range order is described in Sec. III. As an illustrative example, we present results of calculations for a Markov chain in Sec. IV. The application of the ASF to elementary excitations in amorphous solids is discussed in Sec. V, and Sec. VI contains concluding remarks.

II. AUGMENTED SPACE FORMALISM

Let $\{s_j\}$ be a collection of (not necessarily independent) discrete random variables, and $f(s_1, s_2, \ldots)$ some function. We wish to consider the problem of computing $E(f)$, the expected or average value of f,

$$E(f)=\int\int\cdots\int f(s_1, s_2, \ldots)\, P(s_1, s_2, \ldots)\prod_{k=1}^{\infty} ds_k \ , \tag{2.1}$$

where $P(s_1, s_2, \ldots)$ is the joint-probability density function of the variables $\{s_j\}$. When considering elementary excitations in a disordered system, we generally choose f to be a matrix element of the Green's function $(zI-H)^{-1}$ where H is the Hamiltonian and $\{s_j\}$ are the site-occupation variables. The formalism is completely general and for the purpose of discussion it is simpler to consider an arbitrary function.

We assume that each random variable s_j takes on the values $\alpha_1, \ldots, \alpha_N$ and we decompose P into a product of conditional probability densities

$$P(s_1, s_2, \ldots) = p_1(s_1) p_2(s_2/s_1) p_3(s_3/s_1, s_2) \ldots . \tag{2.2}$$

For any joint-probability distribution such a decomposition is always possible. For each density p_j, we construct a Hilbert space ϕ_j of dimension N, and we define the "disorder" space $\Phi = \phi_1 \otimes \phi_2 \otimes \phi_3 \otimes \ldots$, where $\otimes$ denotes direct or tensor product. To each random variable s_j we assign a self-adjoint operator $\tilde{\mathcal{S}}_j$ acting on Φ such that $\tilde{\mathcal{S}}_j \tilde{\mathcal{S}}_k = \tilde{\mathcal{S}}_k \tilde{\mathcal{S}}_j$ for all k and j. To define $\tilde{\mathcal{S}}_j$, we proceed as follows: select a vector v_j^0 in ϕ_j and self-adjoint operators $M_j^{k,l,\ldots m,n}$ on ϕ_j such that

$$p_j(s_j/s_1 = \alpha_k, s_2 = \alpha_l, \ldots, s_{j-2} = \alpha_m, s_{j-1} = \alpha_n) = -\frac{1}{\pi} \lim_{s \to s_j + i0^+} \operatorname{Im}\langle v_j^0 | (sI_j - M_j^{k,l,\ldots,m,n})^{-1} | v_j^0 \rangle , \tag{2.3}$$

where $k, l, \ldots, m, n = 1, 2, \ldots, N$. Such a relation can always be found for any probability density p_j. Note that this says that the eigenvalue distribution of $M_j^{k,l,\ldots,m,n}$ with respect to v_j^0 is precisely p_j. The construction of these operators $M_j^{k,l,\ldots,n}$ is discussed by Mookerjee.[3,4]

We define $\tilde{\mathcal{S}}_1$ by selecting v_1^0 in ϕ_1 and M_1 such that (2.3) holds for $p_1(s_1)$ and then set

$$\tilde{\mathcal{S}}_1 = M_1 \otimes I_2 \otimes I_3 \otimes \cdots , \tag{2.4}$$

where I_j denotes the identity operator on ϕ_j. To define $\tilde{\mathcal{S}}_2$, select v_2^0 in ϕ_2 and self-adjoint operators $M_2^k, k = 1, 2, \ldots, N$, such that (2.3) holds for $p_2(s_2/s_1 = \alpha_k)$, and set

$$\tilde{\mathcal{S}}_2 = \sum_{k=1}^{N} \delta(\alpha_k I_1, M_1) \otimes M_2^k \otimes I_3 \otimes I_4 \otimes \ldots , \tag{2.5}$$

where $\delta(\alpha_k I_1, M_1)$ is the Kronecker δ function. A detailed discussion of the construction of the matrix representation of the δ function is given in Paper I. Similarly

$$\tilde{\mathcal{S}}_3 = \sum_{l=1}^{N} \sum_{k=1}^{N} \delta(\alpha_k I_1, M_1) \otimes \delta(\alpha_l I_2, M_2^k) \otimes M_3^{k,l} \otimes I_4 \ldots , \tag{2.6}$$

where $M_3^{k,l}$ is determined by the choice of v_3^0 in ϕ_3 and the densities $p_3(s_3/s_1 = \alpha_k, s_2 = \alpha_l)$. In general, we define $\tilde{\mathcal{S}}_j$ as

$$\tilde{\mathcal{S}}_j = \sum_{k=1}^{N} \sum_{l=1}^{N} \cdots \sum_{m=1}^{N} \sum_{n=1}^{N} \delta(M_1, \alpha_k I_1) \otimes \ldots \otimes \delta(M_{j-1}^{k,l,\ldots,m}, \alpha_n I_{j-1}) \otimes M_j^{k,l,\ldots,m,n} \otimes I_{j+1} \ldots . \tag{2.7}$$

We note that if the s_i are independent this reduces to the form originally presented by Mookerjee.[3]

Having chosen a vector v_j^0 in ϕ_j for all j we define the vector γ_0 in Φ by $\gamma_0 = v_1^0 \otimes v_2^0 \otimes v_3^0 \otimes \ldots$. The operator $f(\tilde{\mathcal{S}}_1, \tilde{\mathcal{S}}_2, \ldots)$ acts on Φ, and we have

$$E(f) = \langle \gamma_0 | f(\tilde{\mathcal{S}}_1, \tilde{\mathcal{S}}_2, \ldots) | \gamma_0 \rangle . \tag{2.8}$$

This equation is the reason for the previous definitions; it expresses the expected value of f in terms of fixed nonrandom quantities. The calculation of $E(f)$ is now a problem of suitably approximating the inner product.

We have described how the augmented space formalism can handle dependent random variables without providing mathematical proof. In Mookerjee's original papers,[3,4] he gave a heuristic argument which makes it appear that the independence of the random variables is the crucial element in transforming to augmented space. However, by considering the random variables $\{s_j\}$ as defining a distribution on a Hilbert space,[9] it can be shown that the independence is not essential. The mathematical details are discussed in a forthcoming paper.[10]

III. ALLOY

In this section, we use the augmented space formalism to describe the electronic properties of a disordered alloy with short-range order. The formalism is quite general and can be applied equally well to any elementary excitations. We have chosen here to investigate the electronic properties in order to be specific. We describe the configuration of the alloy in terms of the site occupation variables $\{s_i\}$. The site occupation variables describe the type of atom at each site i in the alloy. For example, in a binary alloy composed of A and B atoms, $s_i = s_A(s_B)$ if an A atom (B atom) is present at site i. For alloys with short-range order the $\{s_i\}$ are dependent random variables.

In a disordered system, it is the configurationally averaged quantities that are of physical interest. While the augmented space formalism can be used to evaluate any configurationally averaged quantity, we choose to examine the single-particle Green's function since it is the function most often calculated. For a Hamiltonian H the Green's function is defined by the relation

$$G_{ij}(\{s_n\}) = \langle \psi_i | [zI - H(\{s_n\})]^{-1} | \psi_j \rangle . \tag{3.1}$$

The Hamiltonian is defined on the Hilbert space Ω, and $\{\psi_i\}$ are a set of basis vectors defined in Ω. The configurationally averaged Green's function is defined by the relation

$$\bar{G}_{ij}(z) = \int \int \ldots \int G_{ij}(\{s_n\}) P(\{s_n\}) \prod_{k=1}^{\infty} ds_k , \tag{3.2}$$

where P is the joint probability distribution for the alloy. From (2.1) we see that $\bar{G}_{ij} = E(G_{ij})$ and therefore using Eq. (2.2)–(2.8) we have

$$\bar{G}_{ij} = \langle \gamma_0 | G_{ij}(\tilde{s}_1, \tilde{s}_2, \dots) | \gamma_0 \rangle . \tag{3.3}$$

The only difference is now we are treating elements of a matrix instead of a simple function f. By expanding the space such that a new space $\Sigma = \Omega \otimes \Phi$ which we call the augmented space is created, we can write the configurationally averaged Green's function as

$$\begin{aligned}\bar{G}_{ij} &= \langle \psi_i \otimes \gamma_0 | G(\tilde{s}_1, \tilde{s}_2, \dots) | \psi_j \otimes \gamma_0 \rangle \\ &= \langle \psi_i \otimes \gamma_0 | [zI_\Sigma - H(\tilde{s}_1, \tilde{s}_2, \dots)]^{-1} | \psi_j \otimes \gamma_0 \rangle ,\end{aligned} \tag{3.4}$$

where I_Σ is the identity operator in Σ. In this form we see that we have created a new nonrandom Hamiltonian $H(\tilde{s}_1, \tilde{s}_2, \dots) = \tilde{\mathcal{H}}$ which is defined on the augmented space Σ. $\tilde{\mathcal{H}}$ contains all the physical and statistical information about the alloy. In order to evaluate $\bar{G}_{ij}$ we must invert $zI_\Sigma - \tilde{\mathcal{H}}$. In general this cannot be done exactly so a suitable approximation must be made. As we have discussed in I there are a number of possible approximate methods; the recursion method[5] and the graphical method[6] have been shown to yield Green's functions which are always analytic.[4,7] The failure to produce analytic Green's functions is a major problem of many other theories of disorded systems.[11-13]

The real power of the augmented space formalism lies in the fact that it produces an exact form of the configurationally averaged Green's function which can then be expanded by any of a number of methods to provide an approximation to the Green's function. Since the ASF has transformed the problem into a nonrandom problem, we can use conventional techniques to approximate this new Green's function. For example, using the recursion method on the ASF Green's function we not only produce an averaged Green's function which is analytic but one which has the correct translational symmetry and which provides a good description of the excitations throughout the energy spectrum.

While the theory can be applied to systems of any number of dimensions, as an illustrative example we have chosen to consider in Sec. IV a one-dimensional alloy whose configurations are determined by a Markov process. We first construct the augmented space and then use the recursion method to approximate the electronic density of states.

IV. MARKOV CHAIN

In this section, we investigate the electronic properties of the simplest example of a solid with short-range order—a one-dimensional binary A-B alloy whose configurations are determined by a first order Markov process.[14,15] As previously described, the configurations of the alloy are given in terms of the site occupation variables $\{s_j\}$ which take on the values s_A or s_B depending on whether an A or B atom is present at site j. The lattice sites are labeled relative to some arbitrary site zero. Those to the right are labeled consecutively by the positive integers while those to the left are labeled by the negative integers. We use a nearest-neighbor tight-binding Hamiltonian H to describe the electronic properties of the alloy

$$\begin{aligned} &H_{ij} = e(s_i)\delta_{ij} + W_{ij} , \\ &e(s_i) = e_A\, \delta(s_i, s_A) + e_B\, \delta(s_i, s_B) , \\ &W_{ij} = \begin{cases} W, & |i-j| = 1, \\ 0, & \text{otherwise,} \end{cases} \end{aligned} \tag{4.1}$$

where $H_{ij} = \langle \psi_i | H | \psi_j \rangle$. Note that, since the emphasis of this section is on the treatment of short-range order, we have chosen to consider a Hamiltonian with only diagonal disorder in order to avoid unnecessary complexity. A complete treatment of off-diagonal disorder for a random alloy has already been given in Paper I.

The first-order Markov process is characterized by the transition matrix

$$t = \begin{pmatrix} t_{AA} & t_{AB} \\ t_{BA} & t_{BB} \end{pmatrix} , \tag{4.2}$$

where $t_{\alpha\beta} = p(s_k = s_\beta / s_{k-1} = s_\alpha)$. We construct the Markov chain by starting at the zero site and filling it with an A atom with probability c_A or a B atom with probability $c_B = 1 - c_A$. c_A is equal to the fraction of A atoms in the chain. We fill the sites to right one by one by using the transition matrix t repetitively as follows: once we have determined the type of atom at site 0 we use t to determine the occupation of site 1. From the atom in site 1 we use t to determine the occupation of site 2 and so on. The sites to the left of zero are filled in exactly the same manner except with t redefined for lefthand neighbors, $t_{\alpha\beta} = p(s_k = s_\beta / s_{k+1} = s_\alpha)$. Once the construction is completed the initial site cannot be identified. For a chain defined in this manner the joint probability distribution can be written

$$\begin{aligned} P(\dots, s_{-2}, s_{-1}, s_0, s_1, s_2, \dots) &= p_{-2}(s_{-2}/s_{-1})p_{-1}(s_{-1}/s_0) \\ &\quad \times p_0(s_0)p_1(s_1/s_0)p_2(s_2/s_1)\dots . \end{aligned} \tag{4.3}$$

We can now construct the augmented space as described in Secs. II and III. We define the "disorder" space $\Phi = \ldots \otimes\phi_{-2}\otimes\phi_{-1}\otimes\phi_0\otimes\phi_1\otimes\ldots$ where ϕ_j is a two-dimensional Hilbert space, and the vector $\gamma_0 = \ldots \otimes v_{-2}^0\otimes v_{-1}^0\otimes v_0^0\otimes v_1^0\otimes\ldots$, where $v_j^0 = \binom{1}{0}$ for all j. On ϕ_j we find a self-adjoint operator M_j^α such that

$$p_j(s_j/s_{j-1} = s_\alpha) = -\frac{1}{\pi}\lim_{s\to s_j + i0^+} \operatorname{Im}\langle v_j^0|(sI_j - M_j^\alpha)^{-1}|v_j^0\rangle, \quad (4.4)$$

where $j > 0$. ($j < 0$ is treated similarly.)
Since we have described a stationary Markov process, $p_j = p$. Using the definition of the transition matrix t we have

$$M_j^\alpha = \begin{pmatrix} a^\alpha & b^\alpha \\ b^\alpha & c^\alpha \end{pmatrix},$$

$$a^\alpha = s_A t_{\alpha A} + s_B t_{\alpha B}, \quad (4.5)$$

$$b^\alpha = (s_A - s_B)(t_{\alpha A} t_{\alpha B})^{1/2},$$

$$c^\alpha = s_A + s_B - a^\alpha,$$

where $\alpha = A$ or B. We can now define the operators $\{\tilde{\mathcal{S}}_j\}$ which correspond to the random variables $\{s_j\}$:

$$\vdots$$

$$\tilde{\mathcal{S}}_{-1} = \sum_{\alpha=A}^{B} \cdots I_{-2}\otimes M_{-1}^\alpha \otimes \delta(s_\alpha I_0, M_0)\otimes I_1 \cdots,$$

$$\tilde{\mathcal{S}}_0 \cdots I_{-2}\otimes I_{-1}\otimes M_0 \otimes I_1 \otimes \cdots,$$

$$\tilde{\mathcal{S}}_1 = \sum_{\alpha=A}^{B} \cdots I_{-1}\otimes \delta(s_\alpha I_0, M_0)\otimes M_1^\alpha \otimes I_2 \otimes \cdots, \quad (4.6)$$

$$\tilde{\mathcal{S}}_2 = \sum_{\alpha=A}^{B}\sum_{\beta=A}^{B} \cdots I_{-1}\otimes \delta(s_\alpha I_0, M_0) \otimes\delta(s_\beta I_1, M_1^\alpha)\otimes M_2^\beta \otimes I_3 \cdots,$$

$$\vdots$$

$$\tilde{\mathcal{S}}_j = \sum_{\alpha=A}^{B}\cdots\sum_{\gamma=A}^{B}\sum_{\eta=A}^{B} \cdots I_{-1}\otimes\delta(s_\alpha I_0, M_0) \otimes\cdots\otimes\delta(s_\eta I_{j-1}, M_{j-1}^\gamma) \otimes M_j^\eta \otimes I_{j+1} \cdots,$$

$$\vdots$$

where I_j is the identity operator on ϕ_j. Using the above definitions of the $\{\tilde{\mathcal{S}}_j\}$ and γ_0 along with Eq. (4.1), we can now use (3.4) to write the augmented space representation for the configurationally averaged Green's function

$$\overline{G}_{ij} = \langle \psi_i \otimes \gamma_0 |[zI_\Sigma - H(\tilde{\mathcal{S}}_1, \tilde{\mathcal{S}}_2 \ldots)]^{-1}|\psi_j \otimes\gamma_0\rangle. \quad (4.7)$$

We wish to calculate the electronic density of states $n(\epsilon)$ of the Markov chain which is given by

$$n(\epsilon) = -\frac{1}{\pi}\lim_{z\to\epsilon + i0^+} \operatorname{Im}\overline{G}_{00}(z). \quad (4.8)$$

This is accomplished by applying the recursion method of Haydock, Heine and Kelly[5] to the augmented space construction given above. The recursion method which is based on the Lanczos procedure for inverting matrices[16] generates a continued fraction approximation to the Green's function. The accuracy of the approximation is determined by the number of levels of the continued fraction which are evaluated exactly. For n levels the contributions from the first $2n$ moments are included exactly while the effects of higher moments are approximated in terms of the first $2n$ moments. This method is particularly attractive since it always generates an analytic Green's function. A more detailed discussion of the application of the recursion method to augmented space operators is given in Sec. III of Paper I.

We have performed calculations for Markov chains with $e_A = 3.0$, $e_B = -3.0$, $W = 1.0$, and $c_A = c_B = 0.5$. In Figs. 1–5, the densities of states for these chains calculated using the augmented space formalism and a recursion level of 8 are compared with essentially exact results obtained using the Schmidt method[17] on chains of 100 000 atoms for $t_{BB} = 0.1, 0.3, 0.5, 0.7,$ and 0.9, respec-

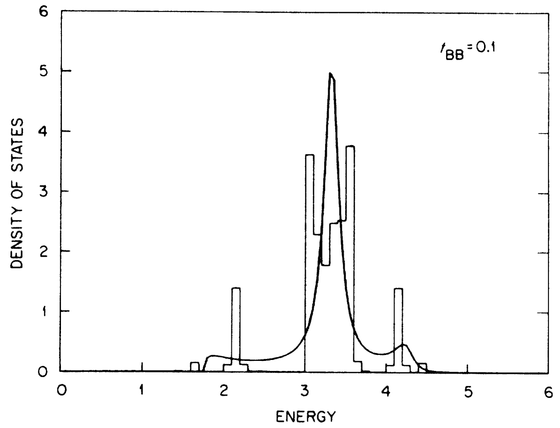

FIG. 1. Comparison of the density of states calculated in the augmented space formalism with a recursion level of 8 (smooth curve) with the corresponding exact calculation (histogram) for a 100 000 atom chain. The parameters of the one-dimensional electronic alloy are $e_A = -e_B = 3.0$, $W = 1.0$, $c_A = 0.5$, and $t_{BB} = 0.1$. In Figs. 1–5, only the transition probability t_{BB} is varied.

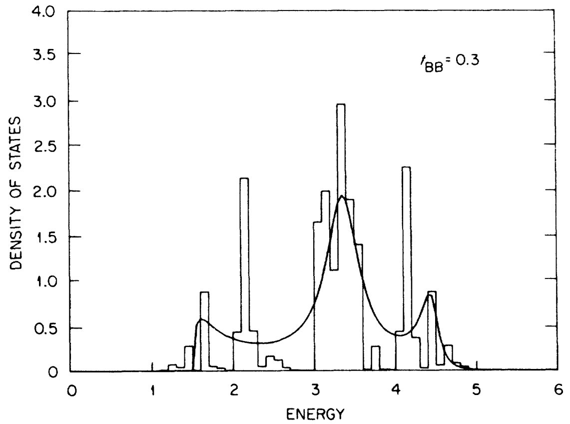

FIG. 2. Density of states as in Fig. 1 with $t_{BB} = 0.3$.

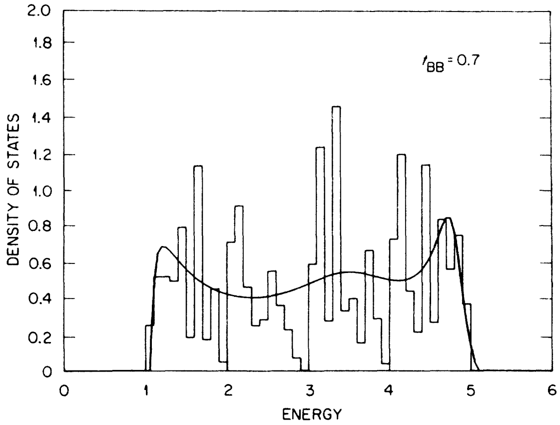

FIG. 4. Density of states as in Fig. 1 with $t_{BB} = 0.7$.

tively. Since the distributions are symmetric about zero for $c_A = 0.5$, we have plotted the results for positive energies only. The theory agrees reasonably well with the exact results throughout the entire spectrum. The theory correctly predicts the band width and the major peaks in the density of states. For t_{BB} small like atoms tend not to be near one another and the resulting structure in the density of states is very sharp. At $t_{BB} = 0.5$ the short-range order is destroyed and we have a completely random chain. As t_{BB} increases above 0.5 the like atoms begin to cluster. In the limit as $t_{BB} \rightarrow 1$, the density of states reduces to the sum of two independent bands, one for the A atoms and one for the B atoms.

V. AMORPHOUS SOLID

In this section, we outline how the ASF can be applied to an amorphous solid. While formally this application is straightforward, certain computational complexities result which makes the use of the ASF for these problems more difficult.

The construction of the augmented space representation of an amorphous solid is conceptually very similar to that of an alloy with short-range order. The difference lies in the fact that we must treat dependent random variables which have a continuous distribution instead of a discrete one. For the purpose of illustration let us consider the electronic properties of a monatomic amorphous solid. We describe the configuration of the amorphous solid in terms of the components of the atomic position vectors $\{r_{i\alpha}\}$ where i is the site index and $\alpha = 1, 2$, or 3 is the cartesian coordinate index.

We wish to determine the configurationally averaged Green's function. For a Hamiltonian H defined on the Hilbert space Ω,

$$\bar{G}_{ij}(z) = \int\int\ldots\int \langle\psi_i|[z - H\{r_{i\alpha}\}]^{-1}|\psi_j\rangle \times P(\{r_{i\alpha}\}) \prod_{k=1}^{\infty}\prod_{\beta=1}^{3} dr_{k\beta}, \qquad (5.1)$$

where $\{\psi_i\}$ are a set of basis vectors defined in Ω, and P is the joint probability density. As in

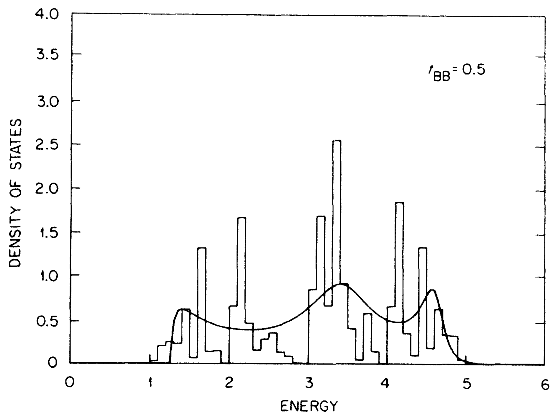

FIG. 3. Density of states as in Fig. 1 with $t_{BB} = 0.5$.

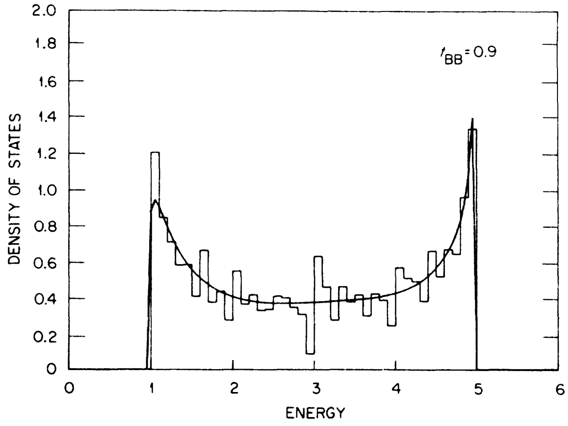

FIG. 5. Density of states as in Fig. 1 with $t_{BB} = 0.9$.

(2.2), we decompose P into a product of conditional probability densities

$$P(r_{11}, r_{12}, r_{13}, r_{21}, \ldots) = p_1(r_{11}) p_2(r_{12}/r_{11}) p_3(r_{13}/r_{11}, r_{12}) \times p_4(r_{21}/r_{11}, r_{12}, r_{13}) \ldots . \quad (5.2)$$

Under appropriate assumptions these conditional probabilities can be defined.[18] In order to construct the augmented space operators which correspond to the continuous random variables we proceed as in Sec. II except now we replace the N dimensional space ϕ_j by infinite dimensional spaces. For each p_j, we construct a Hilbert space ϕ_j of infinite dimension and define the "disorder" space $\Phi = \phi_1 \otimes \phi_2 \otimes \phi_3 \otimes \ldots$. To each random variable $r_{i\alpha}$ we assign a self-adjoint operator $\tilde{\mathfrak{R}}_{i\alpha}$ acting on Φ. $\tilde{\mathfrak{R}}_{i\alpha}$ is defined by selecting a vector v_j^0 in ϕ_j and a self-adjoint operator $M_j(u, v, \ldots, w)$ on ϕ_j such that

$$p_j(r_{i\alpha}/r_{11} = u, r_{12} = v, \ldots) = -\frac{1}{\pi} \lim_{r \to r_{i\alpha} + i0^+} \operatorname{Im} \langle v_j^0 | [rI_j - M_j(u, v, \ldots)]^{-1} | v_j^0 \rangle , \quad (5.3)$$

where $-\infty < u, v, \ldots < +\infty$. Such a relation can always be found for any probability p_j and the construction of the $M_j(u, v, \ldots)$ is discussed by Mookerjee.[3,4] Following the procedure discussed in Sec. II we construct the operators $\tilde{\mathfrak{R}}_{i\alpha}$ as follows:

$$\begin{aligned} \tilde{\mathfrak{R}}_{11} &= M_1 \otimes I_2 \otimes I_3 \otimes \ldots , \\ \tilde{\mathfrak{R}}_{12} &= \int du\, \delta(uI_1, M_1) \otimes M_2(u) \otimes I_3 \ldots , \\ \tilde{\mathfrak{R}}_{13} &= \int\!\!\int du dv\, \delta(uI_1, M_1) \\ &\quad \otimes \delta[vI_2, M_2(u)] \otimes M_3(u, v) \otimes I_4 \ldots , \end{aligned} \quad (5.4)$$

etc.

The only difference between these definitions for $\tilde{\mathfrak{R}}_{i\alpha}$ and those for $\tilde{\mathfrak{S}}_j$ given in Eqs. (2.4)–(2.6) is that we must integrate over continuous variables instead of summing over discrete ones. If we define the augmented space Σ as we have done for the alloy, we have $\Sigma = \Omega \otimes \Phi$, $\gamma_0 = v_1^0 \otimes v_2^0 \otimes v_3^0 \otimes \ldots$, and the configurationally averaged Green's function can be written

$$\overline{G}_{ij} = \langle \psi_i \otimes \gamma_0 | [zI_\Sigma - H(\tilde{\mathfrak{R}}_{11}, \tilde{\mathfrak{R}}_{12}, \ldots)]^{-1} | \psi_j \otimes \gamma_0 \rangle . \quad (5.5)$$

Once again the problem is reduced to finding suitable approximations for inverting $zI_\Sigma - H\{\tilde{\mathfrak{R}}_{i\alpha}\}$). The methods which are described for the alloy problem can be used for the amorphous solid as well and the discussion at the end of Sec. III is applicable here.

While it is a relatively straightforward procedure to formally construct the augmented space for an amorphous solid, it is considerably more difficult to use the formalism for computational purposes than it is for the alloy. Computational problems arise because in Eq. (5.4) we must treat integrals instead of sums and because we must find spectral representations of infinite dimensional M matrices instead of finite ones. As a result, it will be necessary to use some approximate methods such as approximating the integral as a finite sum in constructing the augmented space. The exact nature of these approximations will be strongly dependent on the particular form of the joint probability distribution under consideration.

In the special case of independent random variables, these computational difficulties can be avoided. Mookerjee[4] has calculated the electronic density of states for a three-dimensional system which has a diagonally disordered Hamiltonian which is a function of independent continuous random variables using the special form of the augmented space formalism for independent variables. While an amorphous solid must be described by dependent rather than independent random variables, this example serves as a good illustration of the use of infinite dimensional matrices to represent continuous random variables.

Finally, we note that following a similar procedure we can construct an augmented space representation for a liquid. Of course for the liquid the interactions between particles are time dependent so the operators in augmented space will be functions of time as well.

VI. CONCLUSION

In this paper we have presented a general theory for elementary excitations in disordered systems. This theory is able to treat short-range order as well as off-diagonal and diagonal disorder and yet has none of the short comings which have plagued many earlier theories such as nonanalytic Green's functions or loss of translational invariance. The theory is based on a new mathematical technique for averaging functions of dependent random variables which we call the augmented space formalism. We have included example calculations for first-order Markov chains to illustrate the use of this formalism. Calculations for real three-dimensional problems will be presented in a subsequent paper.

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[1] T. Kaplan and L. J. Gray, J. Phys. C 9, L303-7 (1976).

[2] T. Kaplan and L. J. Gray, Phys. Rev. B 14, 3462 (1976).

[3] A. Mookerjee, J. Phys. C 6, L205 (1973).

[4] A. Mookerjee, J. Phys. C 6, 1340 (1973).

[5] R. Haydock, V. Heine, and M. J. Kelly, J. Phys. C 5, 2845 (1972); 5, 2591 (1975).

[6] P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[7] A. R. Bishop and A. Mookerjee, J. Phys. C 7, 2165 (1974).

[8] A. Mookerjee, J. Phys. C 8, 1524 (1975).

[9] L. Gross, *Analysis in Function Space*, edited by W. T. Martin and I. Segal (MIT Press, Cambridge, Mass., 1963), p. 51.

[10] L. J. Gray and T. Kaplan (unpublished).

[11] B. G. Nickel and W. H. Butler, Phys. Rev. Lett. 30, 363 (1973).

[12] F. Ducastelle, J. Phys. C 7, 1795 (1974).

[13] J. Mertsching, Phys. Status Solidi B 63, 241 (1974).

[14] S. Karlin and H. M. Taylor, *A First Course in Stochastic Processes*, 2nd ed. (Academic, New York, 1975).

[15] R. D. Painter and W. M. Hartman, Phys. Rev. B 10, 2159 (1974).

[16] C. Lanczos, J. Res. Natl. Bur. Stand. 45, 255 (1950).

[17] H. Schmidt, Phys. Rev. 105, 425 (1957).

[18] R. von Mises, *Mathematical Theory of Probability and Statistics* (Academic, New York, 1964), p. 144.