

Rigorous Bound on the Integrated Density of States of a Three-Dimensional Random Alloy*

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(Received 13 June 1973)

We study the lattice model of a random alloy whose Hamiltonian is $\mathcal{H} = -\sum_{r,\delta} t a_r^\dagger a_{r+\delta} + \sum_r \epsilon_r a_r^\dagger a_r$, where δ are nearest-neighbor vectors and ϵ_r is a random site-diagonal energy uniformly distributed over the interval $0 \leq \epsilon_r \leq W$. We prove that the integrated density of states per site $N^{-1} Z(E)$ satisfies the inequality, $N^{-1} Z(E) \leq C_1 e^{-C_2/E}$, where C_1 and C_2 are constants.

I. INTRODUCTION

Recently, much theoretical¹ and experimental² efforts have gone into understanding the many-body properties of alloys. In this paper we study the simplest theoretical model of such an alloy, namely, one in which the hopping matrix elements are periodic, as in a pure system, but in which the site-diagonal energies are random variables. In particular, we study the case when these site-diagonal energies are uniformly distributed over the range of energy from 0 to W . According to the well-known argument of Lifshitz,³ one expects to realize arbitrarily large regions where the site-diagonal energies are arbitrarily close to zero. This reasoning shows that the addition of such random potentials does not change the location of the low-energy band edge. Lifshitz's argument leads to the estimate for the density of states, $\rho(E)$, at energies just above the band edge (taken to be at zero energy),

$$\rho(E) \sim e^{-K/E^{3/2}}, \quad (1)$$

where K is a constant.

In many ways the alloy problem resembles that of phase transitions. Recently, Ma⁴ has attempted to apply the renormalization-group arguments of Wilson⁵ to this problem. His result, in marked disagreement with that, [Eq. (1)] of Lifshitz, is

$$\rho(E) \sim E^\beta, \quad (2)$$

where the critical index β is found to be about 0.80.

Inasmuch as Lifshitz's argument is physically so appealing, we have sought to give a rigorous proof of his estimate. Indeed, in one dimension his estimate becomes $\rho(E) \sim e^{-K'/E^{1/2}}$ and this result has been rigorously confirmed by Eggarter.⁶ Although we have not been able to prove Lifshitz's result in the three-dimensional case, we have obtained rigorously the weaker result that there exists an energy E_0 such that

$$N^{-1} Z(E) \leq C_1 e^{-C_2/E}, \quad E < E_0 \quad (3)$$

where C_1 and C_2 are constants and $N^{-1} Z(E)$ is the in-

tegrated density of states per site:

$$N^{-1} Z(E) = \int_0^E \rho(E') dE'. \quad (4)$$

In view of the form of Eqs. (1) and (3) we define a critical index γ through

$$-\ln Z(E) \sim E^{-\gamma}, \quad E \rightarrow 0. \quad (5)$$

Then our work yields the rigorous lower bound $\gamma \geq 1$ whereas Lifshitz's argument suggests that $\gamma = \frac{3}{2}$. In fact, Lifshitz's value is a rigorous upper bound.

II. PROOF OF BOUND

The model we consider is described by the Hamiltonian

$$\mathcal{H}_R = -\sum_{r,\delta} t a_r^\dagger a_{r+\delta} + \sum_r \epsilon_r a_r^\dagger a_r, \quad (6)$$

where $a_r^\dagger$ creates an excitation at the lattice site at r . For convenience we treat a simple cubic lattice in the form of a rectangular parallelepiped with N_x , N_y , and N_z lattice sites on its three edges. In Eq. (6), δ is summed over the nearest-neighbor vectors of the r th site. We do not introduce periodic boundary conditions, so that sites on the boundary of the system have fewer neighbors than those in the interior. Also, in Eq. (6) ϵ_r is a random site-diagonal energy. We assume that each ϵ_r is an independent random variable governed by a bounded probability distribution, i.e., one for which

$$p(\epsilon) = 0 \quad \text{for } \epsilon < \epsilon_L \text{ or } \epsilon > \epsilon_G \quad (7)$$

and for which $p(\epsilon)$ is bounded for $\epsilon_L < \epsilon < \epsilon_G$. For simplicity we set

$$p(\epsilon) = W^{-1}, \quad 0 < \epsilon < W \quad (8a)$$

$$p(\epsilon) = 0, \quad \text{otherwise.} \quad (8b)$$

From what follows it will become clear that the assumption of this special form for $p(\epsilon)$ is inessential to our arguments. We will study the density of single-particle states of $\mathcal{H}_R$, i.e., those for which $\sum_r a_r^\dagger a_r = 1$. Accordingly, it is immaterial as to whether the a_r 's obey Fermi or Bose statistics.

It is convenient to shift the zero of energy, so that the band edge, when all the ϵ_r 's vanish, occurs at zero energy. We therefore study the Hamiltonian

$$\mathcal{H}(\{\epsilon_r\}) = \sum_{r, \delta} t a_r^\dagger (a_r - a_{r+\delta}) + \sum_r \epsilon_r a_r^\dagger a_r. \quad (9)$$

Furthermore, it is convenient to study the integrated density of states $Z(E)$. For a fixed set of ϵ_r 's, $Z(E, \{\epsilon_r\})$ is defined to be the number of single-particle states of $\mathcal{H}(\{\epsilon_r\})$ having energy less than E . Ultimately, we are interested in the configurationally averaged density of states $Z(E)$, given as

$$Z(E) = \int Z(E, \{\epsilon_r\}) \prod_r [p(\epsilon_r) d\epsilon_r]. \quad (10)$$

Our proof of Eq. (3) involves repeated use of the following theorem.⁷

Let H and H' be two $N \times N$ Hermitian matrices such that

$$H = H' + V, \quad (11)$$

where V is a non-negative $N \times N$ Hermitian matrix, and let $Z(E)$ and $Z'(E)$ be their respective integrated density of eigenvalues. Then the set of eigenvalues of H' are lower bounds for those of H , or equivalently,

$$Z(E) \leq Z'(E). \quad (12)$$

Here a non-negative operator V is one which can be written in bra-ket notation in the form

$$V = \sum_n |n\rangle v_n \langle n|, \quad v_n \geq 0. \quad (13)$$

We now divide the total system of lattice sites into subsystems. That is, if Ω denotes the lattice sites of the system, we write

$$\Omega = \sum_i \Omega_i, \quad (14)$$

where Ω_i denotes the lattice sites of the i th subsystem, which consists of a parallelepiped of sites having N_{xi} , N_{yi} , and N_{zi} sites on its three edges. We now show that

$$Z_\Omega(E) \leq \sum_i Z_{\Omega_i}(E), \quad (15)$$

where the subscript on the single-particle density of states indicates the system of sites to which it pertains. To prove Eq. (15) we write

$$\mathcal{H}_\Omega = \sum_i \mathcal{H}_{\Omega_i} + \sum_{i,j} V_{ij}, \quad (16)$$

in the notation of Eq. (15). Here the Hamiltonian of the i th subsystem is

$$\mathcal{H}_{\Omega_i} = \sum_{r \in \Omega_i} \sum_{\delta} t a_r^\dagger (a_r - a_{r+\delta}) + \sum_{r \in \Omega_i} \epsilon_r a_r^\dagger a_r, \quad (17)$$

where, as in Eq. (6), we do not impose periodic boundary conditions. The interaction between subsystems is of the form

$$V_{ij} = \sum_{\substack{r \in \Omega_i \\ r' \in \Omega_j}}' t (a_r^\dagger - a_{r'}^\dagger) (a_r - a_{r'}), \quad (18)$$

where the double prime indicates that only terms for which r and r' are nearest neighbors are to be included. Clearly V_{ij} is non-negative in the sense of Eq. (13). Hence, according to the theorem, dropping the interaction terms in Eq. (16) cannot decrease the density of states. However, in the absence of these interaction terms the density of single-particle states is simply the sum of the densities of states of the subsystems. Thus Eq. (15) is proved.

For simplicity we now introduce an inequality in terms of a discrete probability distribution for the ϵ_r 's. According to the theorem we can write

$$Z(E, \{\epsilon_r\}) \leq Z(E, \{\delta_r\}), \quad (19)$$

if $\delta_r \leq \epsilon_r$ for all r . Now we apply Eq. (19) by taking, for each r ,

$$\delta_r = 0 \quad \text{if} \quad 0 < \epsilon_r < a, \quad (20a)$$

$$\delta_r = a \quad \text{if} \quad a < \epsilon_r < W. \quad (20b)$$

Use of Eqs. (19), (20), and (8) allows us to write

$$Z(E) \leq \sum_{\{\sigma_r\}} Z(E, \{\delta_r\}) \prod_r \hat{p}(\delta_r), \quad (21)$$

where the σ 's are summed over the two values 0 and a , and

$$\hat{p}(0) = a/w \quad (22a)$$

$$\hat{p}(a) = 1 - \hat{p}(0). \quad (22b)$$

To bound $Z(E)$ for small E we choose the subsystems to be as large as possible within the restriction that

$$A''/N_i > E, \quad (23)$$

where N_i is the number of sites in the i th subsystem and A'' is the constant in Eq. (A10). Thus, we write

$$\frac{1}{2} A''/E < N_i < A''/E. \quad (24)$$

Furthermore, we consider energies small enough that N_i is large enough for the bounds in Eq. (A10) to hold. With this construction it is clear that the lowest single-particle energy level of any subsystem having one or more nonzero σ 's has an energy greater than E , so that for such subsystems $Z(E, \{\sigma_r\}) = 0$. Since only subsystems having all σ 's zero contribute to Eq. (15) we may write

$$Z_\Omega(E) \leq \sum_i (a/w)^{N_i} Z_{\Omega_i}(E, \{\sigma_r = 0\}). \quad (25)$$

We need to evaluate $Z_{\Omega_i}(E, \{\sigma_r = 0\})$, which is the density of states of the unperturbed Hamiltonian, i. e., that of Eq. (17) with all $\epsilon_r = 0$. The single-particle energies for this case are readily found to be

$$E_{l,m,n} = t \left(6 - 2 \cos \frac{l\pi}{N_{xi}} - 2 \cos \frac{m\pi}{N_{yi}} - 2 \cos \frac{n\pi}{N_{zi}} \right), \quad (26)$$

where l , m , and n are integers satisfying $0 \leq l < N_{xi}$; $0 \leq m < N_{yi}$; and $0 \leq n < N_{zi}$. Apart from E_{000} the lowest single-particle energy level occurs for either l , m , or n equal to 1 and is of order $N^{-2/3}$. Since $N^{-2/3} \gg N^{-1}$, we see that for sufficiently large N we may set $Z_{\Omega_i}(E, \{\sigma_r = 0\}) = 1$. This evaluation, together with the inequality of Eq. (24), shows that Eq. (25) implies that there exists an E_0 such that

$$N^{-1}Z_{\Omega}(E) \leq C_1 e^{(A'/E) \ln(a/W)}, \quad \text{for } E < E_0, \quad (27)$$

where C_1 is a constant. This result is equivalent to that stated in Eq. (3).

III. DISCUSSION

The variational principle can be used to obtain upper bounds for the energies and thence lower bounds for $Z(E)$. Use of Lifshitz's wave functions as trial functions shows that his result, [Eq. (1)], is a lower bound for $Z(E)$.

ACKNOWLEDGMENTS

The author would like to thank Dr. B. Nickel for stimulating my interest in this problem. I also appreciate the helpful comments of Dr. R. Stinchcombe and Professor R. Weinstock.

APPENDIX A: MINIMUM ENERGY FOR SINGLE-DEFECT POTENTIAL

In this Appendix we obtain rigorously a formula for the minimum single-particle energy in the presence of a single-defect potential. To do this, we use the well-known⁸ procedure of solving the Schrödinger eigenvalue problem by constructing the Green's function

$$G_E(r, r') = \sum_n \frac{\psi_n^*(r) \psi_n(r')}{E - E_n}, \quad (A1)$$

where $\psi_n(r)$ is the n th eigenfunction with energy eigenvalue E_n when all but one of the σ 's in Eq. (17) are zero. In particular, we take $\sigma_{r''} = a$, so that there is a site-diagonal repulsive potential at that site of strength a . In the absence of defect potentials, the Green's function, denoted $G_E^0(r, r')$, is

$$G_E^0(r, r') = \sum_n \frac{[\psi_n^0(r)]^* \psi_n^0(r')}{(E - E_n^0)} \quad (A2)$$

where $\psi_n^0(r)$ and E_n^0 are the n th eigenfunction and eigenvalue, respectively, in this case.

We may express G in terms of G^0 as

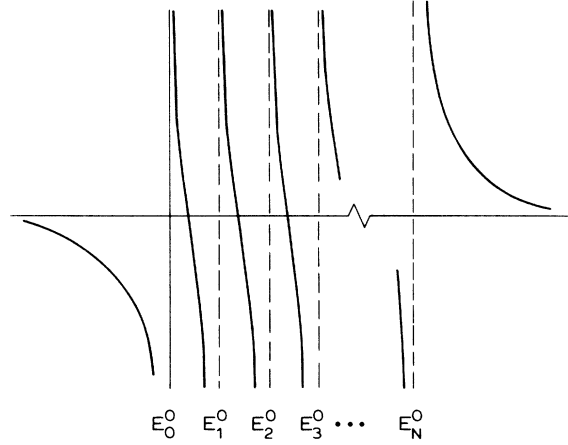


FIG. 1. Schematic behavior of $G_E^0(r'', r'')$.

$$G_E(r, r') = G_E^0(r, r') + G_E^0(r, r'') t G_E^0(r'', r'). \quad (A3)$$

Here we have introduced the t matrix, which satisfies

$$t = a + a G_E^0(r'', r'') t, \quad (A4)$$

and thus is

$$t = a [1 - a G_E^0(r'', r'')]^{-1}. \quad (A5)$$

Based on the fact that the poles of $G_E(r, r')$ yield the eigenvalues, an analysis of Eqs. (A3) and (A5) shows that eigenvalues occur when (i) $E = E_n^0$, in the case when E_n^0 is a degenerate eigenvalue of the system in the absence of defect potentials, or (ii) when $1 = a G_E^0(r'', r'')$, i. e., when

$$a^{-1} = G_E^0(r'', r'') = \sum_n \frac{|\psi_n^0(r'')|^2}{E - E_n^0}. \quad (A6)$$

To find the minimum single-particle eigenvalue we need only consider case (ii), i. e., Eq. (A6). Since $G_E^0(r'', r'')$ has poles at E_n^0 , and since $dG_E^0(r'', r'')/dE$ is negative for $E \neq E_n^0$, the right-hand side of Eq. (A6) has the familiar form shown in Fig. 1.

The discussion in Appendix B shows that for a three-dimensional system E_∞ , the minimum single-particle energy for $a = \infty$, i. e., for an infinite potential at r'' , is of order N^{-1} :

$$NE_\infty \sim g_0(r'')^{-1}, \quad N \rightarrow \infty \quad (A7)$$

where $g_0(r'')$ is defined in Eq. (B4a). For finite a it is clear that $E < E_\infty$. A treatment similar to that leading to Eq. (B3) shows that for a three-dimensional system the minimum single-particle energy for finite a , denoted E_a , obeys the inequality

$$(1 - \gamma \epsilon) g_0(r'') \geq (NE_a)^{-1} - a^{-1} \geq g_0(r''), \quad (A8)$$

where $\epsilon = NE_\infty$ and γ is of the order $N^{-1/3}$. Thus, for sufficiently large N we have that E_a is of order N^{-1} :

$$NE_a \sim [a^{-1} + g_0(r'')]^{-1}, \quad N \rightarrow \infty. \quad (\text{A9})$$

In particular, Eq. (A8) shows that for $a > 0$ and for sufficiently large N there exists a nonzero A'' such that

$$E_a \geq A''/N. \quad (\text{A10})$$

APPENDIX B: PROOF THAT E_∞ IS OF ORDER N^{-1}

In this Appendix we show that E_∞ is of order N^{-1} for large N . We define E_∞ as the lowest single-particle energy when the defect potential at r'' is infinite. As discussed in Appendix A, the eigenvalue condition, in this case, may be written

$$\sum_n \frac{|\psi_n^0(r'')|^2}{E_\infty - E_n^0} = 0, \quad 0 \leq E_\infty \leq E_1^0, \quad (\text{B1})$$

where E_1^0 is the energy of the next-to-lowest energy eigenvalue of the perfect crystal. It is clear from Fig. 1 that a solution to Eq. (B1) does exist and is unique. We now set $E_\infty = \epsilon/N$, and note that the lowest-energy eigenvalue and eigenvector of the perfect crystal are, respectively, $E_0^0 = 0$ and $\psi_0^0(r) = N^{-1/2}$, whence we may write

$$\frac{1}{\epsilon} = \sum_n' \frac{|\psi_n^0(r'')|^2}{E_n^0 - \epsilon/N}, \quad (\text{B2})$$

where the prime indicates that the lowest-energy term which gives rise to the left-hand side of Eq. (B2) is to be omitted from the summation. Since $E_1^0 - \epsilon/N$ must be positive, we have the inequality

$$(1 - \gamma\epsilon)^{-1} g_0(r'') \geq \epsilon^{-1} \geq g_0(r''), \quad (\text{B3})$$

where

$$g_0(r'') = \sum_n' \frac{|\psi_n^0(r'')|^2}{E_n^0} \quad (\text{B4a})$$

and

$$\gamma = (NE_1^0)^{-1}. \quad (\text{B4b})$$

We may write Eq. (B3) as

$$(1 - \gamma\epsilon) g_0(r'')^{-1} \leq \epsilon \leq g_0(r'')^{-1}. \quad (\text{B5})$$

For one- and two-dimensional systems, $g_0(r)$ diverges in the limit $N \rightarrow \infty$. We will adopt the simple, although perhaps over-restrictive, definition of a three-dimensional system as one for which N_x/N_y and N_y/N_z remain of order unity as $N \rightarrow \infty$. With this definition it is straightforward to establish bounds for $g_0(r)$ for a three-dimensional system of the form

$$0 < A \leq g_0(r) \leq B < \infty, \quad (\text{B6})$$

where A and B are constants independent of N and r for sufficiently large N . Then since $E_1^0 \sim N^{-2/3}$, Eqs. (B4b), (B5), and (B6) imply that for sufficiently large N ,

$$(1 - A'/N^{1/3}) \leq \epsilon g_0(r'') \leq 1, \quad (\text{B7})$$

where A' is a constant, independent of N and r .

From Eq. (B7) we conclude that

$$NE_\infty \sim g_0(r'')^{-1}, \quad N \rightarrow \infty. \quad (\text{B8})$$

*Work supported in part by the National Science Foundation.

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