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Impurity-Band Tails in the High-Density Limit. II. Higher Order Corrections

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In an earlier paper, I, the authors presented a theory of the low-energy tail of an electron band in a semiconductor in the presence of a high density of impurities. This theory was based on the approximation that all the local potential fluctuations binding states of a given energy have the same shape. We now discuss corrections to the density of states $\rho(E)$ and the spectral density $A(\mathbf{k},E)$ by treating the difference between the actual random potential and the average well shape as a small perturbation. An *average higher-order energy* correction to the density of states is proposed, which displaces all energies by the average difference between the perturbed and unperturbed energies, and the calculation of this correction is discussed for the limiting case of a random potential obeying Gaussian statistics. We also discuss the *complete* second-order correction proposed by Zittartz and Langer, which leads to the exact asymptotic form of $\rho(E)$ in a Gaussian potential, and we show how the formulas can be extended to impurity potentials of nonzero range. For three-dimensional Gaussian models, the approximate density of states of our earlier paper had the form $\rho(E) \sim \xi^{-2}A(E)\exp[-B(E)/(2\xi)]$, where ξ is a parameter proportional to the density of impurities and to the square of the strength of the individual impurity potentials. The corrections described in the present paper modify the function $A(E)$, but not $B(E)$. We also discuss briefly corrections to the momentum dependence of our earlier approximation to the spectral density $A(\mathbf{k},E)$.

1. INTRODUCTION

In an earlier paper,[1] the authors presented an approximate method for calculating the density of states $\rho(E)$, and the momentum-dependent spectral density, $A(\mathbf{k},E)$, in the low-energy tail of an electron band of a semiconductor, in the presence of a high density of impurities. The states in the low-energy tail are bound in wells in the random potential, arising from large fluctuations in the local density of impurities. The assumption used in I was that all the eigenstates at a given energy in the tail have the same shape, or equivalently, that all the corresponding potential wells have the same shape. This assumption is not exact, of course; it is only a first approximation. In fact, the approximation leads to a small overestimate of the energy of each eigenstate, and an underestimate of the density of states.

In the present paper, we shall discuss methods for improving the approximation of I. In principle, we may calculate the correct energy of each eigenstate from perturbation theory, using as a zeroth-order potential the "typical well shape" of I, and using as a perturbation the difference between the actual random potential and the typical shape. The "average higher-order energy correction" described in Sec. 3 of the present paper changes the approximate density of states by displacing every energy calculated in I by the expectation value of the energy correction due to the difference between the true Hamiltonian and the unperturbed Hamiltonian. In the limit of an infinite density of impurities, where the random potential may be described by Gaussian statistics, third and higher terms in perturbation theory make no contribution to the density of states in the low-energy tail, and the average higher-order correction may be calculated explicitly, as shown in Sec. 4.

When the bulk of this paper was essentially completed, the authors received a preprint of a very interesting paper by Zittartz and Langer,[2] which studies the low-energy tail of the density of states of a particle in a Gaussian-white-noise potential in one, two, and three dimensions. The method of ZL, in effect, exactly includes the second-order correction to the unperturbed energy, including *fluctuations* of the energy correction about its expectation value. In Sec. 5 of the present paper we rederive the ZL results from our own point of view, and show how a slight generalization of ZL can be used to calculate the complete second-order correction for Gaussian potentials other than white noise (i.e., where the impurity potentials have nonzero range).

In I, we calculated an approximate density of states for a one-dimensional model of an infinite density of weak point scatterers, (a white-Gaussian-noise potential), for which the density of states is known exactly. The approximate density of states $\rho_1(E)$ was found to be $(1/\sqrt{5})\rho_{\mathrm{as}}(E)$ where $\rho_{\mathrm{as}}(E)$ is the asymptotic form in the tail of the exact density of states. With the average-second-order correction, given in (4.23) of the present paper, the density of states $\rho_2(E)$ is found to be $0.92\ \rho_{\mathrm{as}}(E)$. When the fluctuations in the second-order correction are included, the resulting approximation, $\rho_d(E)$, to the density of states becomes $\rho_{\mathrm{as}}(E)$ itself, as was explicitly verified by Zittartz and Langer. Indeed, as we emphasize at the beginning of Sec. 5, this result, $\rho_d(E)=\rho_{\mathrm{as}}(E)$, verified for a one-dimensional potential with delta-function autocorrelation can be expected to be valid for any Gaussian potential, including three-

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[1] B. I. Halperin and M. Lax, Phys. Rev. **148**, 722 (1966). Hereafter referred to as I.

[2] J. Zittartz and J. S. Langer, Phys. Rev. **148**, 741 (1966). Hereafter referred to as ZL.

dimensional potentials with general autocorrelations of arbitrary range.

The relatively small changes in the density of states, as one goes from $\rho_1(E)$ to $\rho_2(E)$ to $\rho_d(E)$, demonstrates the physical soundness of calculating the density of states, deep in the tail, by the "minimum counting" methods of I.

The assumption in I of a fixed shape for the wave functions at a given energy led at once to an approximation for the form of the momentum dependence of the spectral density $A(\mathbf{k},E)$. Corrections to this form, due to deviations of the wave functions from the uniform shape calculated in I, are discussed briefly in Sec. 6.

2. GENERAL THEORY OF THE LOW-ENERGY TAIL

A. The Model

We shall assume a one-band Hamiltonian for the electron, in which explicit electron-electron effects are replaced by a screened Coulomb interaction. The impurities are represented by a model potential that includes the proper effective intraband matrix elements of the original Hamiltonian. We shall write the one-electron Hamiltonian in the form

$$\mathcal{H}=\mathcal{T}+V(\mathbf{x}), \tag{2.1}$$

where $\mathcal{T}$ is a "kinetic energy" operator, equal to the sum of the energy of the electron in the pure host crystal plus the average potential of the impurities, and where $V(\mathbf{x})$ represents the fluctuations of the total impurity potential about its mean value. The potential $V(\mathbf{x})$ is a random function which depends on the positions of all the impurities.[3]

We shall assume that the wave functions vary slowly from one lattice site to the next, so that the kinetic energy has an effective-mass form, and the position variable $\mathbf{x}$ may be treated as a continuous variable.

The density of states $\rho(E)$ is defined by

$$\rho(E)\equiv\frac{1}{\Omega}\left\langle\sum_i \delta(E-E_i)\right\rangle, \tag{2.2}$$

where E_i is the energy of the ith eigenstate of the Hamiltonian, Ω is the volume of the crystal, and the angular brackets indicate an average over an ensemble of impurity positions.

In the absence of the fluctuating potential $V(\mathbf{x})$; the density of states would vanish for energies below the minimum eigenvalue of $\mathcal{T}$, which we denote by E_0. The low-energy tail of the actual system occurs when E is sufficiently lower than E_0 so that an unusually large negative fluctuation in $V(\mathbf{x})$ is required to bind a state with energy E. The required negative fluctuation or "well" in $V(\mathbf{x})$ may be caused by an unusually large local density of attractive impurities, or by an unusually small local density of repulsive impurities.

B. The First Approximation

The central assumption of I was that all the eigenstates, at a *given energy E* in the low-energy tail, have the same shape. In other words, we assume that for all eigenstates ψ_i, such that $E_i\approx E$, we have

$$\psi_i(\mathbf{x})\approx f(\mathbf{x}-\mathbf{x}_i), \tag{2.3}$$

where f is a fixed function which depends in a continuous way on the parameter E. The point $\mathbf{x}_i$, the "center" of the ith wave function, will be different, of course, for each state. The wave function ψ_i will be localized in the crystal in the vicinity of a potential well of the correct size to bind a wave function of the prescribed energy E. We are interested here in the case of a high concentration of impurities; this means that there will be many impurities within the range of the wave function ψ_i, or many impurities which contribute to the corresponding potential well.

We shall suppose, for the moment, that the form of the function $f(\mathbf{x})$ is known for the given value of the energy E.

The function $f(\mathbf{x}-\mathbf{y})$ can be used[4] to define a variational energy $E_f(\mathbf{y})$, which is the matrix element of the Hamiltonian $\mathcal{H}$ in the state $f(\mathbf{x}-\mathbf{y})$:

$$E_f(\mathbf{y})=\int f(\mathbf{x}-\mathbf{y})\mathcal{H}f(\mathbf{x}-\mathbf{y})d\mathbf{x}. \tag{2.4}$$

The variational energy is itself the sum of two terms

$$E_f(\mathbf{y})=\theta+V_s(\mathbf{y}), \tag{2.5}$$

where

$$\theta=\int f(\mathbf{x}-\mathbf{y})\mathcal{T}f(\mathbf{x}-\mathbf{y}), \tag{2.6}$$

$$V_s(\mathbf{y})\equiv\int f(\mathbf{x}-\mathbf{y})^2V(\mathbf{x})d\mathbf{x}. \tag{2.7}$$

The kinetic-energy term θ is independent of the choice of $\mathbf{y}$, whereas the ("smoothed") potential term V_s is an average of the random potential $V(\mathbf{x})$ in a certain region centered about $\mathbf{y}$, and will depend on the choice of $\mathbf{y}$. The function $V_s(\mathbf{y})$ may be thought of as a smoothed version of the original potential and will

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[3] Although we speak of the particle in our problem as an "electron," the same model may be used to describe holes in a valence band. A similar model may also be used to describe tightly bound excitons interacting with a random thermal deformation potential in a lattice of infinitely massive atoms. Application of the methods of I and the present paper to the exciton case are discussed in B. I. Halperin, Ph.D. thesis, University of California, Berkeley, 1965 (unpublished).

[4] It is always possible to choose the eigenfunctions of $\mathcal{H}$ to be real, and we shall therefore assume f to be real. We also require that f be properly normalized, and, for the sake of uniqueness, that f have its maximum where its argument equals zero.

exhibit a large negative fluctuation in each region where there is an unusually large local concentration of attractive impurities or small local concentration of repulsive impurities, that is, in each region which binds a low-energy eigenstate.

If (2.3) is assumed to hold, then the points $\mathbf{x}_i$ which are the centers of wave functions ψ_i with $E_i \approx E$ must satisfy

$$E_f(\mathbf{x}_i) \approx E. \tag{2.8}$$

Furthermore, it was shown in I, that $\mathbf{x}_i$ must be a point such that $E_f(\mathbf{y})$ is a local *minimum* at $\mathbf{x}_i$. [The reason for this is that (2.4) is a *variational* estimate of the ground-state energy of the local potential well. We are always interested in the local *ground* state, because potential wells strong enough to bind a wave function in the low-energy tail will be few and far between; the probability of finding two overlapping wells, or of finding one isolated well so deep that we must consider the first *excited* state of the well, is negligibly small.] One also finds that there will be only one local minimum in E_f for each deep potential well and thus there will be a bound state ψ_i at *each* local minimum satisfying (2.8). It, therefore, follows from assumption (2.3) that the density of states at energy E is equal to the expectation value of the number of local minima in $E_f(\mathbf{y})$, per unit volume, such that E_f at the minimum falls in a unit energy interval about E.

Let $\{\mathbf{y}_j\}$ be the set of all points such that $E_f(\mathbf{y})$ is a local minimum at $\mathbf{y}=\mathbf{y}_j$. Then the density of states which corresponds to the assumption (2.3) may be written

$$\rho_f(E) \equiv \langle \delta[E-E_f(\mathbf{y})] \sum_j \delta(\mathbf{y}-\mathbf{y}_j) \rangle. \tag{2.9}$$

[The result for $\rho_f(E)$ is, of course, independent of the choice of $\mathbf{y}$, as long as the system is statistically homogeneous.]

If the random potential $V(\mathbf{x})$ is the sum of potentials due to independent, randomly distributed impurities, the quantity $\rho_f(E)$ can be evaluated with a computer, for any given function f. Thus the approximate density of states could be calculated, if the correct function f were known for each value of E.

As was shown in I, the best choice of f is that which maximizes the value of $\rho_f(E)$.[5] The fact that $E_f(\mathbf{x}_i)$ is equal to or larger than the true energy E_i, together with the fact that the density of states in the tail decreases rapidly with decreasing energy, implies that

$$\rho_f(E) \leq \rho(E). \tag{2.10}$$

The equality sign in (2.10) would hold only if $E_f(\mathbf{x}_i)=E_i$ for all the wave functions with $E_i \approx E$, i.e., if assumption (2.3) were exact for the function f in question. Although (2.3) will not be exact, we get the best possible approximation to the true density of states by choosing f to maximize $\rho_f(E)$. Thus we have the approximation

$$\rho_1(E) \equiv \max_f \rho_f(E). \tag{2.11}$$

The function f chosen in this way will be a function for which the difference $|\psi_i(\mathbf{x})-f(\mathbf{x}-\mathbf{x}_i)|$ is, on the average, as small as possible, and f may be interpreted as the "average" or "typical" shape for the wave functions at energy E. The choice of f will be different for each value of E.

C. The Difference between the Exact and Variational Energies

In order to improve our approximation for the density of states, we must consider the difference between the variational energy $E_f(\mathbf{x}_i)$ and the true energy E_i of the corresponding eigenstate. It is convenient to define a function $p(E'|E)$ which is the conditional probability that $E_i=E'$, when it is known that $E_f(\mathbf{x}_i)=E$, where f is the function which maximizes $\rho_f(E)$.

At energies deep in the low-energy tail, the one-to-one correspondence between eigenstates and minima in $E_f(\mathbf{y})$ will be extremely good. It is therefore essentially exact in the low-energy tail to write

$$\rho(E') = \int p(E'|E)\rho_1(E)dE. \tag{2.12}$$

The essential step in finding an improved approximation to the density of states is to make a good approximation for $p(E'|E)$. If the difference $|\psi_i(\mathbf{x})-f(\mathbf{x}-\mathbf{x}_i)|$ is generally small as we believe, it is logical to try to simplify the problem somewhat by using a perturbation expansion in which $f(\mathbf{x}-\mathbf{x}_i)$ is the unperturbed wave function.

Let us define the function $V_0(\mathbf{x})$ by

$$V_0(\mathbf{x}) \equiv [(E-\mathcal{T})f(\mathbf{x})]/f(\mathbf{x}), \tag{2.13}$$

so that

$$[\mathcal{T}+V_0(\mathbf{x}-\mathbf{x}_i)]f(\mathbf{x}-\mathbf{x}_i) = Ef(\mathbf{x}-\mathbf{x}_i). \tag{2.14}$$

The assumption that an eigenstate $\psi_i(x)$ has the form $f(\mathbf{x}-\mathbf{x}_i)$ and energy $E_i=E$, is equivalent to the assumption that the true potential $V(\mathbf{x})$ is equal to $V_0(\mathbf{x}-\mathbf{x}_i)$ in the neighborhood of $\mathbf{x}_i$. Assumption (2.3) is thus equivalent to the assumption that all the potential wells which bind a state of a given energy E have exactly the same form, $V_0(\mathbf{x}-\mathbf{x}_i)$. Although (2.3) is not exact, it is still true that the function $V_0(\mathbf{x})$, corresponding to the function f which maximizes $\rho_f(E)$, should be in some sense the "average shape" of potential wells which bind an eigenstate of energy E. If (2.3) is a good approximation, then the deviations of the potential wells from their average shape will be small. We shall therefore expand the difference E_i

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[5] We shall assume here that this choice of f is unique. The complications which occur if this is not the case are discussed in I.

$-E_f(\mathbf{x}_i)$ in powers of the perturbation $V(\mathbf{x})-V_0(\mathbf{x}-\mathbf{x}_i)$. We write

$$E_i=E+\epsilon_1+\epsilon_2+\epsilon_3+\cdots, \tag{2.15}$$

where ϵ_n is of order $(V-V_0)^n$. The first term may be written

$$\begin{aligned}\epsilon_1&\equiv\int f(\mathbf{x}-\mathbf{x}_i)[V(\mathbf{x})-V_0(\mathbf{x}-\mathbf{x}_i)]f(\mathbf{x}-\mathbf{x}_i)d\mathbf{x}\\&=V_s(\mathbf{x}_i)-[E-\theta].\end{aligned}\tag{2.16}$$

The condition that $E_f(\mathbf{x}_i)=E$ implies that ϵ_1 vanishes.

The second-order term in the perturbation expansion (2.15) may be written

$$\begin{aligned}\epsilon_2\equiv\int f(\mathbf{x}-\mathbf{x}_i)&[V(\mathbf{x})-V_0(\mathbf{x}-\mathbf{x}_i)]\hat{G}(\mathbf{x}-\mathbf{x}_i,\,\mathbf{x}'-\mathbf{x}_i)\\&\times[V(\mathbf{x}')-V_0(\mathbf{x}'-\mathbf{x}_i)]f(\mathbf{x}'-\mathbf{x}_i)d\mathbf{x}d\mathbf{x}',\end{aligned}\tag{2.17}$$

where $\hat{G}$ is a "modified Green's function" of the unperturbed Hamiltonian, defined by[6]

$$[E-\mathcal{T}-V_0(\mathbf{x})]\hat{G}(\mathbf{x},\mathbf{x}')=\delta(\mathbf{x}-\mathbf{x}')-f(\mathbf{x})f(\mathbf{x}'). \tag{2.18}$$

We may also write down expressions for ϵ_3 and higher terms. When Gaussian statistics are applicable, however, we shall find that ϵ_3 and higher terms are negligible in the low-energy tail, and it suffices to consider ϵ_2.

3. AVERAGE HIGHER-ORDER ENERGY CORRECTION

A. Definition

The simplest way to include some of the effects of the difference between the true energy E_i and the variational energy $E_f(\mathbf{x}_i)$ is to correct all energies by the *average value* of the difference between E_i and $E_f(\mathbf{x}_i)$.

Let us use double angular brackets with subscript E to indicate the conditional expectation value of a random variable, when it is known that E_f has a local minimum at $\mathbf{y}$ with $E_f(\mathbf{y})=E$. Thus for any random variable γ, we have

$$\langle\langle\gamma\rangle\rangle_E\equiv\langle\gamma\delta[E-E_f(\mathbf{y})]\textstyle\sum_j\delta(\mathbf{y}-\mathbf{y}_j)\rangle[\rho_1(E)]^{-1} \tag{3.1}$$

where y_j are defined as in (2.9), and where f is the function which maximizes $\rho_f(E)$. The conditional probability distribution $p(E'|E)$, defined in Sec. 2C, is expressed in the form $\langle\langle\gamma\rangle\rangle_E$ by

$$p(E'|E)=\langle\langle\delta(E'-E_i)\rangle\rangle_E, \tag{3.2}$$

where E_i is the exact energy of the eigenstate corresponding to the local minimum at $\mathbf{y}$.

We define the "average higher-order energy," $S(E)$, by

$$S(E)\equiv\langle\langle E_i-E\rangle\rangle_E. \tag{3.3}$$

Then we may define an approximation ρ_2 to the density of states, which includes a correction for the "average higher-order energy shift" $S(E)$, by inserting the approximation

$$p(E'|E)\approx\delta[E'-E-S(E)] \tag{3.4}$$

in (2.12). We obtain

$$\rho_2[E+S(E)]=\rho_1(E)dE/d[E+S(E)]. \tag{3.5}$$

Since we shall find that $dS(E)/dE$ is small compared to 1 in the low-energy tail, we shall replace the derivative on the right-hand side of (3.5) by unity. In most cases, it turns out that S is sufficiently small so that we may neglect the difference between $S(E)$ and $S[E-S(E)]$. In this case:

$$\rho_2(E)\approx\rho_1[E-S(E)]. \tag{3.6}$$

Even if $S(E)$ is small, however, there may be a significant fractional difference between $\rho_2(E)$ and $\rho_1(E)$, because ρ_1 is a rapidly varying function of its argument.

The difficult step in the evaluation of ρ_2 is the calculation of the quantity $S(E)$. By expanding E_i-E in the perturbation series (2.15), we see that $S(E)$ is determined by the conditional expectation values $\langle\langle V(\mathbf{x})\rangle\rangle_E$, $\langle\langle V(\mathbf{x})V(\mathbf{x}')\rangle\rangle_E$, etc., the first n functions being required to evaluate $\langle\langle\epsilon_n\rangle\rangle_E$. If the random potential $V(\mathbf{x})$ is the sum of potentials due to independent randomly scattered impurity atoms, it is possible, in principle, to calculate each of these conditional expectation values. The calculations are extremely difficult, however, except in the very high density limit, where one may use Gaussian statistics for the random potential $V(\mathbf{x})$. It is probable that the calculation of $S(E)$ will not be practical except under the Gaussian assumption. Further details of the calculation in the Gaussian case will be given in Sec. 4.

B. Relation to the Exact Density of States

We know that E_i is always smaller than $E_f(\mathbf{x}_i)$, and therefore $S(E)$ is always negative. Since the density of states increases with increasing energy, $\rho_2(E)$ will always be bigger than $\rho_1(E)$. Nevertheless, $\rho_2(E)$ will still be smaller than the true density of states $\rho(E)$, deep in the low-energy tail, as we may see by the following argument.

Let us first note that the probability distribution

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[6] An alternative definition of $\hat{G}$ may put (2.17) in a more familiar form. We know that f is the ground state of a particle in the well $V_0(x)$. Let the excited states be denoted by $\Phi_v(x)$, $v=1, 2, \cdots$, and let the corresponding energies be denoted by ω_v. The energies ω_v form a continuum for energies greater than E_0, and may include one or more bound states between E and E_0. The function $\hat{G}$ can now be written $\hat{G}(\mathbf{x},\mathbf{x}')=\sum_v[\Phi_v(\mathbf{x})\Phi_v(\mathbf{x}')]/(E-\omega_v)$.

$p(E'|E)$ must satisfy the relations

$$\int p(E'|E)dE'=1, \tag{3.7}$$

$$\int p(E'|E)E'dE'=E+S(E). \tag{3.8}$$

If the magnitude of $E_i-E_f(\mathbf{x}_i)$ is always a small correction to the energy difference $E_f(\mathbf{x}_i)-E_0$, then the conditional probability $p(E'|E)$ will be a much more rapidly varying function of the difference $E'-E$ than of the sum $E+E'$. Accordingly in (2.12), we may replace $p(E'|E)$ by $p(2E'-E|E')$. We may now use (3.7) and (3.8) to put (2.12) in the form

$$\rho(E')=\rho_1[E'-S(E')]+\int p(2E'-E|E') \times\{\rho_1(E)-\rho_1[E'-S(E')]-[E-E'+S(E')] \times\rho_1'[E'-S(E')]\}dE, \tag{3.9}$$

where ρ_1' is the first derivative of ρ_1. If $\rho_1(E)$ is concave upwards in the region of integration, as it must be if the low-energy tail is smooth, then the integrand in (3.9) is non-negative. Using (3.6) we find that

$$\rho(E')>\rho_2(E'). \tag{3.10}$$

4. GAUSSIAN STATISTICS

A. The Approximation $\rho_1(E)$

We shall now discuss in greater detail the case in which the random potential $V(\mathbf{x})$ obeys Gaussian statistics. The statistical properties of a set of Gaussian variables with mean zero are completely determined by the second moments of the distribution. The properties of $V(\mathbf{x})$ are thus determined by the autocorrelation function $\langle V(\mathbf{x})V(\mathbf{x}')\rangle$. It is convenient to write

$$\langle V(\mathbf{x})V(\mathbf{x}')\rangle\equiv\xi W(\mathbf{x}-\mathbf{x}'), \tag{4.1}$$

where the parameter ξ is proportional to the concentration of impurities and to the square of the strength of the individual impurities, and where the function $W(\mathbf{x}-\mathbf{x}')$ depends only on the shapes of the impurity potentials, and may be normalized in any convenient fashion. (See discussion in I for further details.)

An energy E will be in the low-energy tail if E_0-E is large compared with the fluctuations in the smoothed potential $V_s(\mathbf{x})$. Thus, as discussed in I, the terms that are important for properties of the low-energy tail in a Gaussian potential are those which are important in the limit $\xi\rightarrow 0$, when the energy E is held fixed. Except for terms which are negligible in this limit, the approximate density of states ρ_f is given by Eq. (3.23) of I:

$$\rho_f(E)=\frac{\sigma_1\sigma_2\sigma_3}{(2\pi)^2}\frac{(\theta-E)^3}{\xi^2\sigma_0^7}\exp\left[-\frac{(\theta-E)^2}{2\xi\sigma_0^2}\right], \tag{4.2}$$

where

$$\sigma_0^2\equiv\int f(\mathbf{x})^2W(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')^2d\mathbf{x}d\mathbf{x}', \tag{4.3}$$

and where σ_1^2, σ_2^2, and σ_3^2 are the three eigenvalues of the tensor

$$\mathbf{K}\equiv-\int f(\mathbf{x}')^2W(\mathbf{x}-\mathbf{x}')\nabla\nabla f(\mathbf{x})^2d\mathbf{x}'d\mathbf{x}. \tag{4.4}$$

The matrix $\mathbf{K}$ is symmetric and positive definite. The three coordinate axes can always be chosen so that $\mathbf{K}$ is diagonal and the eigenvalues are the diagonal elements. In the case of spherical symmetry, the matrix $\mathbf{K}$ is proportional to the unit tensor, and it is only necessary to evaluate one diagonal component.[7]

In the low-energy tail, the important factor on the right-hand side of (4.2) is the exponential factor. When trying to find the function f which maximizes ρ_f, it suffices to use the function f which maximizes the expression

$$\Gamma(E,f)=(\theta-E)^2/\sigma_0^2. \tag{4.5}$$

Application of variational calculus to (4.5), leads to a differential equation for f of the form (2.14), $[\mathcal{T}+V_0]f=Ef$, with $V_0(\mathbf{x})$ itself given by

$$V_0(\mathbf{x})=-\mu\int W(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')^2d\mathbf{x}'. \tag{4.6}$$

In (4.6), μ is a Lagrange multiplier which is determined by the requirement that $\int f(\mathbf{x})^2d\mathbf{x}=1$. The value of μ is related to θ and σ_0 by

$$\mu=(\theta-E)/\sigma_0^2, \tag{4.7}$$

as shown in I, Eq. (5.17).

The pair of Eqs. (2.14) and (4.6) may be solved for $f(\mathbf{x})$ and μ by an iterative procedure described in I. Numerical results for screened Coulomb interactions have been plotted in I. The approximate density of states ρ_1 is obtained when this function f is used to evaluate the quantities θ, σ_0, σ_1, σ_2, and σ_3, that appear in (4.2).

Note that the function f, and consequently the quantities θ, σ_0, etc., depend on the energy E, but are independent of the strength parameter ξ. For three-dimensional models, the function $\rho_1(E)$ therefore has the form

$$\rho_1(E)=\xi^{-2}A(E)\exp[-B(E)/2\xi], \tag{4.8}$$

where $A(E)$ and $B(E)$ are independent of ξ.

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[7] Formula (4.2) is given for the case of a three-dimensional model. For one-dimensional models, ρ_f contains an exponential factor identical to that in (4.2), but the form of the prefactor is different than in the three-dimensional case.

B. Conditional Expectation Values

We shall now develop some techniques necessary for the calculation of corrections to the density of states $\rho_1(E)$ for Gaussian models. Note that the logarithmic derivative of $\rho(E)$ behaves like ξ^{-1}, in the limit $\xi \to 0$. When computing corrections to the density of states due to the difference between E_i and $E_f(\mathbf{x}_i)$, we may therefore neglect all terms in the energy shift which are of higher order than the first power in the parameter ξ; the percentage error in the density of states due to such terms will disappear in the limit of small ξ. As we shall see shortly, this means that we need only keep the leading term in $E_i - E_f(\mathbf{x}_i)$.

In order to evaluate the average-higher-order-energy correction, we must calculate conditional expectation values of the form $\langle\langle\gamma\rangle\rangle_E$. Using relation (3.4) of I, we may write definition (3.1), of the present paper, in the form

$$\langle\langle\gamma\rangle\rangle_E = \frac{\langle\gamma\delta[E-E_f(\mathbf{y})]\delta[\boldsymbol{\nabla} V_s(\mathbf{y})]\det\boldsymbol{\nabla\nabla} V_s(\mathbf{y})\rangle}{\langle\delta[E-E_f(\mathbf{y})]\delta[\boldsymbol{\nabla} V_s(\mathbf{y})]\det\boldsymbol{\nabla\nabla} V_s(\mathbf{y})\rangle}. \tag{4.9}$$

We may also define a different conditional expectation value $\langle\langle\gamma\rangle\rangle^E$ by

$$\langle\langle\gamma\rangle\rangle^E = \frac{\langle\gamma\delta[E-E_f(\mathbf{y})]\delta[\boldsymbol{\nabla} V_s(\mathbf{y})]\rangle}{\langle\delta[E-E_f(\mathbf{y})\delta[\boldsymbol{\nabla} V_s(\mathbf{y})]\rangle}. \tag{4.10}$$

The new quantity $\langle\langle\gamma\rangle\rangle^E$ is the conditional expectation value of the variable γ, when it is given that $V_s(\mathbf{y}) = E-\theta$, and $\boldsymbol{\nabla} V_s(\mathbf{y})=0$. The difference between $\langle\langle\gamma\rangle\rangle^E$ and $\langle\langle\gamma\rangle\rangle_E$ arises from the weighting factor $\det\boldsymbol{\nabla\nabla} V_s(\mathbf{y})$ which is present in the latter. As shown in I, this determinant is equal to a constant, $(\theta-E)^3\sigma_1{}^2\sigma_2{}^2\sigma_3{}^2/\sigma_0{}^6$, plus a random term whose deviations from zero will be of order $\xi^{1/2}$, when it is known that $E_f(\mathbf{y})=E$. Thus, to lowest order in ξ, we may cancel the weighting factor $\det\boldsymbol{\nabla\nabla} V_s(\mathbf{y})$ from the numerator and denominator of (4.9), and we may write

$$\langle\langle\gamma\rangle\rangle_E \approx \langle\langle\gamma\rangle\rangle^E. \tag{4.11}$$

Conditional expectation values of the form $\langle\langle\gamma\rangle\rangle^E$ are relatively simple to evaluate because they involve only linear constraints. Under linear constraints, the conditional probability distribution of $V(\mathbf{x})$ is still Gaussian, and all the properties of the conditional distribution are determined by the first two moments. These moments may be evaluated by the methods of I, Appendix A. We find for the first moment;

$$\begin{aligned}\langle\langle V(\mathbf{x})\rangle\rangle^E &= [\langle V(\mathbf{x})V_s(\mathbf{y})\rangle/\langle V_s(\mathbf{y})^2\rangle](E-\theta)\\ &= V_0(\mathbf{x}-\mathbf{y}).\end{aligned} \tag{4.12}$$

Thus the conditional expectation value of the random potential $V(\mathbf{x})$, in the vicinity of the local minimum in the smoothed potential, is given by the "unperturbed potential" $V_0(\mathbf{x}-\mathbf{y})$. This confirms our earlier remarks that V_0 represents some kind of "average shape" of the potential wells which bind a state with energy E.

Using again the methods of I, Appendix A, we find that

$$\begin{aligned}\langle\langle[V(\mathbf{x})-V_0(\mathbf{x}-\mathbf{y})][V(\mathbf{x}')-V_0(\mathbf{x}'-\mathbf{y})]\rangle\rangle^E\\ = \xi w(\mathbf{x}-\mathbf{y},\, \mathbf{x}'-\mathbf{y}),\end{aligned} \tag{4.13}$$

where

$$\begin{aligned}w(\mathbf{x},\mathbf{x}') &= W(\mathbf{x}-\mathbf{x}')\\ &\quad -\frac{V_0(\mathbf{x})V_0(\mathbf{x}')}{\mu^2\sigma_0{}^2}-\sum_{\alpha=1}^{3}\frac{[\nabla_\alpha V_0(\mathbf{x})][\nabla_\alpha V_0(\mathbf{x}')]}{\mu^2 K_{\alpha\alpha}}.\end{aligned} \tag{4.14}$$

The summation in (4.14) is over the three coordinate directions, and the axes are assumed to have been chosen so that the tensor $\mathbf{K}$ is diagonal.

We see that the "perturbing potential" $[V(\mathbf{x}) - V_0(\mathbf{x}-\mathbf{y})]$ is of order $\xi^{1/2}$. The second-order energy ϵ_2 is thus of order ξ, the term ϵ_3 is of order $\xi^{3/2}$, etc. It follows that for a random potential obeying Gaussian statistics, only the term ϵ_2 need be considered in the density of states.

Note that the situation is more complicated if we cannot assume Gaussian statistics for $V(\mathbf{x})$. In this case, there is no simple parameter, comparable to ξ, which tells us rigorously which terms are important in the low-energy tail. It will still be true that $\langle\langle V(\mathbf{x})\rangle\rangle_E$ is approximately $V_0(\mathbf{x}-\mathbf{y})$, and the conditional root-mean-square deviation of $V(\mathbf{x})$ will be relatively small in many cases. However, even if ϵ_2 is small, it is not necessarily true that ϵ_3 and higher terms are proportionately smaller still. If $V(\mathbf{x})$ does not obey Gaussian statistics, the higher moments of the distribution are not determined by the first two moments. In particular, although the perturbing potential $[V(\mathbf{x})-V_0(\mathbf{x}-\mathbf{y})]$ is small on the average there may be regions where it is large. If we are dealing with a finite density of impurities, such regions can occur in the neighborhood of each impurity site. A region of strong perturbation may make a contribution to ϵ_3, ϵ_4, etc., that is as important as the contribution to ϵ_2. In any case, even the calculation of $\langle\langle\epsilon_2\rangle\rangle^E$ will be difficult for the non-Gaussian situation.

C. Average Higher-Order Energy Correction

We are now in a position to calculate the average higher-order energy correction for the Gaussian case. The average energy difference $S(E)$ will be equal to $\langle\langle\epsilon_2\rangle\rangle^E$, except for terms which are negligible in the limit $\xi\to 0$. An expression for $\langle\langle\epsilon_2\rangle\rangle^E$ can be written immediately from (4.13) and (2.17). We find that

$$S(E) = -\xi C(E), \tag{4.15}$$

where $C(E)$ is independent of ξ and is given by

$$C(E) = -\int f(\mathbf{x})\hat{G}(\mathbf{x},\mathbf{x}')f(\mathbf{x}')w(\mathbf{x}',\mathbf{x})d\mathbf{x}'d\mathbf{x}. \tag{4.16}$$

If ϵ is any quantity of order ξ, it is exact, in the limit $\xi \to 0$, to write

$$\rho_1(E-\epsilon)=\rho_1(E)\exp[\epsilon B'(E)/2\xi], \tag{4.17}$$

where $B'(E)$ is the derivative of the function $B(E)$ of (4.8). We know that $B(E)$ is equal to value of $\Gamma(E,f)$, where Γ is defined by (4.5), and f is chosen to minimize $\Gamma(E,f)$, for the given E. When E is varied, we have

$$dB(E)=(\partial\Gamma/\partial E)dE+(\delta\Gamma/\delta f)\delta f. \tag{4.18}$$

But f has been chosen so that $\delta\Gamma/\delta f=0$. We have therefore

$$B'(E)=(\partial\Gamma/\partial E)=-2\mu, \tag{4.19}$$

where μ is given by Eq. (4.7).

In order to find the corrected density of states $\rho_2(E)$, we substitute (4.15) and (4.17) in (3.6). We find

$$\rho_2(E)=\rho_1(E)\exp[\mu C(E)]. \tag{4.20}$$

The most difficult steps in the numerical evaluation of the average higher-order energy correction are the calculation of the Green's functions $\hat{G}$, and the evaluation of the integrals (4.16) for $S(E)$. In models where W and f are spherically symmetric, these calculations can be simplified by decomposition into spherical harmonics. Calculations are currently under way for the model of an infinite density of weak screened-Coulomb impurity potentials, which will illustrate the computational techniques. (We plan to publish these calculations in Paper IV of the series.)

The average higher-order energy correction to the density of states is a factor which is independent of ξ. The ξ dependence of ρ, is therefore the same as that of ρ_1, given by Eq. (4.8). The function $B(E)$ is the same as before; only the function $A(E)$ is changed. As we shall see in Sec. 5, the exact asymptotic form of $\rho(E)$ still has this form, with a slightly different function $A(E)$.

D. One-Dimensional White-Gaussian-Noise Model

The theory we have developed for the approximation ρ_2 can be applied to the one-dimensional model of a white-Gaussian-noise potential, for which ρ_1 was calculated in I. The white-Gaussian-noise model arises as the limit of an infinite density of weak point scatterers. The potential $V(x)$ obeys Gaussian statistics, with

$$W(x-x')=\tfrac{1}{2}\delta(x-x'). \tag{4.21}$$

It is convenient to choose the unit of mass so that the kinetic energy for the one-dimensional model has the simple form

$$\mathcal{T}=-\tfrac{1}{2}(d^2/dx^2). \tag{4.22}$$

The pair of Eqs. (2.14) and (4.6) can be solved exactly for the function $f(x)$, in the one-dimensional model, and one finds

$$f(x)=(\kappa/2)^{1/2}\operatorname{sech}\kappa x, \tag{4.23}$$

$$\mu=4\kappa, \tag{4.24}$$

where

$$\kappa=(-2E)^{1/2}. \tag{4.25}$$

The approximate density of states ρ_1 was found in I to have the form

$$\rho_1(E)=\frac{1}{\sqrt{5}}\frac{4\kappa^2}{\pi\xi}\exp\left[-\frac{4}{3}\frac{\kappa^3}{\xi}\right]. \tag{4.26}$$

The density of states for the white-Gaussian-noise model can be calculated exactly at all energies by specialized one-dimensional methods, unrelated to the low-energy tail approximations we have discussed here.[8–10] In the low-energy-tail limit, $\xi\to 0$, or $E\to -\infty$, the density of states has the exact asymptotic form

$$\rho_{\mathrm{as}}(E)=\frac{4\kappa^2}{\pi\xi}\exp\left[-\frac{4}{3}\frac{\kappa^3}{\xi}\right]. \tag{4.27}$$

The approximation ρ_1 differs from the exact asymptotic form by a factor $1/\sqrt{5}$.

Equation (2.18), defining the modified Green's function $\hat{G}$, can be solved analytically for the present model. The solution is

$$\begin{aligned}\hat{G}(x,x')&=(\kappa^{-1}/2)\operatorname{sech}\kappa x\operatorname{sech}\kappa x'\\&\quad\times[\kappa x'-\kappa x-\tfrac{1}{2}e^{2\kappa x}-\tfrac{1}{2}e^{-2\kappa x'}],\ \text{for } x'\geq x,\\&=(\kappa^{-1}/2)\operatorname{sech}\kappa x\operatorname{sech}\kappa x'\\&\quad\times[\kappa x-\kappa x'-\tfrac{1}{2}e^{2\kappa x'}-\tfrac{1}{2}e^{-2\kappa x}],\ \text{for } x\geq x'.\end{aligned} \tag{4.28}$$

The conditional correlation function $w(x,x')$ has the form

$$\begin{aligned}w(x,x')&=(1/2)\delta(x-x')-(3/8)\kappa\operatorname{sech}^2\kappa x\operatorname{sech}^2\kappa x'\\&\quad-(15/8)\kappa\operatorname{sech}^2\kappa x\tanh\kappa x\operatorname{sech}^2\kappa x'\tanh\kappa x'.\end{aligned} \tag{4.29}$$

The integrals involved in (4.16) are evaluated in the Appendix to this paper and lead to the result:

$$C(E)=(13/72)\kappa^{-1}. \tag{4.30}$$

It follows that

$$\begin{aligned}\rho_2(E)&=\rho_1(E)\exp[13/18]\\&\approx(0.921)\rho_{\mathrm{as}}(E).\end{aligned} \tag{4.31}$$

Thus we find the result, quoted without proof in I, that the approximate theory of the low-energy tail, including average higher-order energy corrections, reproduces the exact asymptotic form of the density of states except for a uniform error of 8%.

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[8] H. L. Frisch and S. P. Lloyd, Phys. Rev. **120**, 1175 (1960).
[9] B. I. Halperin, Phys. Rev. **138**, A104 (1965).
[10] M. Lax, Rev. Mod. Phys. **38**, 541 (1966), Sec. 4.

E. Divergent Second-Order Corrections

Although it is true that the energy shift $S(E)$ approaches zero, as $\xi\rightarrow 0$, there are some models for which the assumption $|S(E)|\ll\theta-E$ does not become valid until ξ becomes much smaller than the value necessary for the validity of various other parts of our theory. For example, the two- and three-dimensional equivalents of the Gaussian-white-noise model lead to a divergent second-order energy shift due to short-wavelength potential fluctuations, unless the fluctuations are cut off below a certain wavelength. A short-wavelength cutoff is always present if the potential correlation function $W(\mathbf{x}-\mathbf{x}')$ is not truly a δ function, but it is clear that for any given ξ, if the range of $W(\mathbf{x}-\mathbf{x}')$ is sufficiently small, the second-order correction will be very large. The divergent part of the energy shift will be independent of the energy E, however, and we can therefore write

$$S(E)=-\xi[C_0+c(E)], \tag{4.32}$$

where C_0 is a large constant whose value depends on the cutoff in W, and where $|\xi c(E)|$ is independent of the cutoff and may be assumed small compared to $\theta-E$ in the region of interest. In this case, one cannot use (3.6) to define ρ_2 but must go back to (3.5). The most convenient form for the result is

$$\rho_2(E-\xi C_0)\approx\rho_1(E)\exp[\mu c(E)]. \tag{4.33}$$

The function ρ_1 and the quantity μ are convergent in the white-Gaussian-noise limit and are therefore independent of the cutoff.

The term ξC_0 in (4.32) has the effect of displacing the bottom of the band as a whole. An energy E' will be in the low-energy tail, and the approximation $\rho(E')\approx\rho_2(E')$ will only be valid only if E' is less than $E_0-\xi C_0$.

The Gaussian-white-noise limit, in three dimensions, will be discussed in further detail in a future paper (III) in this series.

5. COMPLETE SECOND-ORDER ENERGY CORRECTION IN GAUSSIAN STATISTICS

According to the arguments of Sec. 4B, all terms higher than ϵ_2, in the perturbation expansion for $E_i-E_f(\mathbf{x}_i)$, may be neglected, for the low-energy tail of the density of states in a Gaussian random potential. Consequently, if we could properly include the energy correction ϵ_2 in the density of states, including the statistical fluctuations of ϵ_2 about its expected value, we would expect to reproduce the exact asymptotic form for the density of states.

Zittartz and Langer, in the reference mentioned above,[2] show how the density of states, including the complete second-order energy correction, can, in fact, be evaluated. Although ZL are concerned with the Gaussian-white-noise limit in one, two, or three dimensions, their formulas can be readily extended to any potential correlation function $W(\mathbf{x}-\mathbf{x}')$, as we shall show below. By a series of clever maniuplations, ZL have succeeded in evaluating their formulas analytically for the one-dimensional white-noise model. They indeed obtain the correct asymptotic form (4.27) for $\rho(E)$, including the exact over-all constant.

Although the general analysis of the low-energy tail in ZL is different than that in I and the present paper, their formulas can also be derived from the present point of view. We shall start with formula (2.12) for the exact density of states in the low-energy tail. We must first evaluate the conditional probability distribution $p(E'|E)$. According to the arguments of Sec. 4B, it is correct in the limit $\xi\rightarrow 0$ to set

$$p(E'|E)\approx\langle\langle\delta(E'-E-\epsilon_2)\rangle\rangle^E. \tag{5.1}$$

It will be convenient to assume that the local minimum in the function $E_f(\mathbf{y})$ occurs at $\mathbf{y}=0$.

Let $u(\mathbf{x})$ be any real function such that

$$W(\mathbf{x}-\mathbf{x}')=\int u(\mathbf{x}-\mathbf{z})u(\mathbf{x}'-\mathbf{z})d\mathbf{z}. \tag{5.2}$$

One such function $u(\mathbf{x})$ may be found by taking the inverse Fourier transform of the square root of the Fourier transform of W. If $V(\mathbf{x})$ is the sum of impurity potentials of a single fixed shape, then we may choose $u(\mathbf{x})$ to be proportional to the potential of an isolated impurity.

Let us define a Gaussian random function $N(\mathbf{x})$ such that

$$V(\mathbf{x})=\int u(\mathbf{x}-\mathbf{x}')N(\mathbf{x}')d\mathbf{x}'. \tag{5.3}$$

Equation (4.1) implies that $N(\mathbf{x})$ has the form of white Gaussian noise, with

$$\langle N(\mathbf{x})N(\mathbf{x}')\rangle=\xi\delta(\mathbf{x}-\mathbf{x}'). \tag{5.4}$$

Let $\{\varphi_n(\mathbf{x})\}$, $n=0, 1, 2, \cdots$, be any complete, orthonormal set of real functions. If $N(\mathbf{x})$ is expanded as

$$N(\mathbf{x})=\sum_{n=0}^{\infty}\eta_n\varphi_n(\mathbf{x}), \tag{5.5}$$

then the random variables η_n are independent Gaussian variables with mean zero and variance ξ. It is convenient to choose $\varphi_0(\mathbf{x})$ to be equal to $\sigma_0^{-1}\int u(\mathbf{x}'-\mathbf{x})f(\mathbf{x}')^2d\mathbf{x}'$, and to choose $\varphi_1(\mathbf{x})$, $\varphi_2(\mathbf{x})$, and $\varphi_3(\mathbf{x})$ proportional to the three components of $\nabla\varphi_0(\mathbf{x})$. If the coordinate axes have been chosen so as to diagonalize the tensor $\mathbf{K}$ of (4.4), then the functions φ_0, φ_1, φ_2, and φ_3 will in fact be orthogonal to each other. The value of the smoothed potential at $\mathbf{y}=0$ may be written as

$$V_s(0)=\sigma_0\int\varphi_0(\mathbf{x})N(\mathbf{x})d\mathbf{x}=\sigma_0\eta_0. \tag{5.6}$$

The value of η_0 is therefore fixed, if we require that $V_s(0)=E-\theta$. Similarly we find that the condition $\nabla V_s(0)=0$ requires that η_1, η_2, and η_3 equal 0. On the other hand, because all the remaining functions φ_n will be orthogonal to the first four, the remaining variables η_n will be statistically independent of the values of $V_s(0)$ and $\nabla V_s(0)$.

Inserting (5.5) into (5.3) and (5.3) into (2.17), we can write the second-order energy (2.17) as

$$\epsilon_2=\sum_{m,n=4}^{\infty}\eta_m\eta_n\int\varphi_m(\mathbf{y})I(\mathbf{y},\mathbf{y}')\varphi_n(\mathbf{y}')d\mathbf{y}'d\mathbf{y}\,,\qquad(5.7)$$

where

$$I(\mathbf{y},\mathbf{y}')=\int\int f(\mathbf{x})u(\mathbf{x}-\mathbf{y})\hat{G}(\mathbf{x},\mathbf{x}')\times u(\mathbf{x}'-\mathbf{y}')f(\mathbf{x}')d\mathbf{x}d\mathbf{x}'.\qquad(5.8)$$

The expression (5.7) can be reduced to a diagonal quadratic form by choosing the $\varphi_n(\mathbf{y})$ to be eigenfunctions of $I(\mathbf{y},\mathbf{y}')$, in the subspace orthogonal to φ_0, φ_1, φ_2, and φ_3.[11] More precisely, we must choose φ_n to be eigenfunctions of the operator PIP,

$$PIP\varphi_n(\mathbf{x})=-\alpha_n\varphi_n(\mathbf{x})\,,\qquad(5.9)$$

where P is the projection operator that projects out the states φ_0, φ_1, φ_2, φ_3. The operator P is an integral operator with the kernel

$$P(\mathbf{x},\mathbf{x}')=\delta(\mathbf{x}-\mathbf{x}')-\sum_{n=0}^{3}\varphi_n(\mathbf{x})\varphi_n(\mathbf{x}')\,.\qquad(5.10)$$

Because of the projection operator P, the states φ_0, φ_1, φ_2, φ_3 are trivially eigenfunctions of (5.9) with $\alpha_n=0$. The set $\{\varphi_n\}$ including the first four states is therefore a complete orthogonal set[12] as required. Furthermore, the second-order energy now reduces to the diagonal form:

$$\epsilon_2=-\sum_{n=4}^{\infty}\alpha_n\eta_n^2\,.\qquad(5.11)$$

Using the fact that the η_n are independent Gaussian variables of variance ξ [see (5.4), (5.5)], we can rewrite (5.1) as

$$p(E'|E)=\langle\langle\delta[E'-E-\epsilon_2(\eta)]\rangle\rangle\,,\qquad(5.12)$$

where the average of any function $f(\eta)$ of the η_n is defined by

$$\langle\langle f(\eta)\rangle\rangle=\int\frac{d\eta_4}{(2\pi\xi)^{1/2}}\int\frac{d\eta_5}{(2\pi\xi)^{1/2}}\cdots f(\eta)\exp\left[-\sum_{n=4}^{\infty}\frac{\eta_n^2}{2\xi}\right].\qquad(5.13)$$

From (5.11) and (5.12), we see that [as alleged in Sec. 3B] $p(E'|E)$ is a strong function of $E'-E$, and for fixed $E'-E$, depends only weakly on E, since the only dependence on E is then the relatively small variation of the parameters α_n.

We shall first consider the usual case where ϵ_2 is small. It is then correct to use for the α_n the values appropriate to energy E', rather than the values at E. If we now substitute (5.12) into (2.12), we can perform the integration over E, and we obtain

$$\rho(E')=\langle\langle\rho_1[E'-\epsilon_2(\eta)]\rangle\rangle\,.\qquad(5.14)$$

Dropping the prime on E, and using Eq. (4.17), we may put (5.14) in the form

$$\rho(E)=\rho_1(E)\langle\langle\exp[\mu\epsilon_2(\eta)/\xi]\rangle\rangle\,.\qquad(5.15)$$

All the approximations we have made in deriving (5.15) lead to errors which are negligible in the limit $\xi\rightarrow0$. Thus, evaluating (5.15), we obtain the correct asymptotic form

$$\rho_{\mathrm{as}}(E)=\rho_1(E)\prod_{n=4}^{\infty}\left\{\int(2\pi\xi)^{-1/2}d\eta_n\exp\left[\frac{-\eta_n^2(1-2\mu\alpha_n)}{2\xi}\right]\right\}$$
$$=\rho_1(E)\prod_{n=4}^{\infty}(1-2\mu\alpha_n)^{-1/2}\,.\qquad(5.16)$$

Note that the correction factor in (5.16) is independent of ξ.

The complete second-order-energy correction is determined by the set of eigenvalues of the operator PIP, and by the degeneracy of each eigenvalue.[13] The *average* second-order energy correction is also determined by the α_n. Evaluation of (4.16) for $C(E)$ is equivalent to taking the trace of PIP, and the approximate density of states ρ_2 may be written as

$$\rho_2(E)=\rho_1(E)\exp\left[\mu\sum_{n=4}^{\infty}\alpha_n\right].\qquad(5.17)$$

Comparing (5.16) and (5.17), we find that

$$\rho_{\mathrm{as}}(E)=\rho_2(E)\prod_{n=4}^{\infty}\left[\frac{\exp(-2\alpha_n\mu)}{1-2\alpha_n\mu}\right]^{1/2}.\qquad(5.18)$$

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[11] The transformation from a set of correlated random variables to a set of uncorrelated variables (i.e., in the Gaussian case, independent variables) by introducing eigenfunctions of the autocorrelation function seems to have been introduced first by K. Karhunen [Ann. Acad. Sci. Fennicae Ser. AI **34**, (1946); **37** (1947)]. This procedure has been exploited in the theory of nonlinear random processes by M. Kac and A. J. F. Siegert. See, for example, their early paper [Ann. Math. Statist. **18**, 438 (1947)]. In the present context, this method was used by Zittartz and Langer, Ref. 2. A summary of the method, including certain nonuniqueness features, is presented in Sec. 13 of M. Lax, Rev. Mod. Phys. **32**, 25 (1960).

[12] It is not actually necessary to use P to project out the functions φ_1, φ_2, and φ_3, as they turn out to be eigenfunctions of I in any case. Explicit orthogonalization to the state φ_0 is necessary, however, because φ_0 is not an eigenfunction of I. Equation (5.10) of ZL is actually incorrect, because it does not contain this explicit orthogonalization. ZL do not use their Eq. (5.10) directly, however, but find the eigenfunctions from their Eq. (5.16). By setting the right-hand side of this latter equation equal to zero, they are, in effect, orthogonalizing to φ_0.

[13] In the product (5.16) and in subsequent equations, degenerate eigenvalues are included as many times as they appear in the operator PIP. Our notation differs in this respect from that of ZL.

Equation (5.18) is more convenient for computation than (5.16), as the product in (5.18) converges more rapidly than that in (5.16).

In general, evaluating the trace of an integral operator is much simpler than finding the eigenvalues. The *average* higher-order correction is thus easier to find than the exact asymptotic form. As we found in the example of one-dimensional white noise, the function ρ_2 contains the most important corrections to $\rho_1(E)$. For many purposes $\rho_2(E)$ will be satisfactory, and it will not be worth the additional effort necessary to evaluate ρ_{as}.

The results of ZL, and the results we have just derived, were based on the assumption that ϵ_2 is small. As discussed in Sec. 4E, the second-order energy ϵ_2 will be divergent in the Gaussian-white-noise limit in two and three dimensions. In the white-noise limit, the value of ϵ_2 will exhibit relatively small deviations from a value $-\xi C_0$, where C_0 is a large constant whose value depends on the cutoff in the short-wavelength potential fluctuations. The correct asymptotic formula for the density of states, when $|\epsilon_2+\xi C_0|$ is small while ξC_0 is not, is

$$\rho_{\text{as}}(E-\xi C_0)=\rho_2(E-\xi C_0)\prod_{n=4}^{\infty}\left[\frac{\exp(-2\alpha_n\mu)}{1-2\alpha_n\mu}\right]^{1/2}. \tag{5.19}$$

The μ and α_n which appear in (5.19) are calculated the same way as before from Eqs. (4.7) and (5.9). The function f which occurs implicitly in these equations is the function which maximizes $\rho_f(E)$. The product in (5.19) is convergent in the white-noise limit. The values of μ and α_n are insensitive to the cutoff in W and may be evaluated under the assumption $W(\mathbf{x}-\mathbf{x}')=\delta(\mathbf{x}-\mathbf{x}')$.

The ξ dependence of the density of states in the low-energy tail, in the three-dimensional white-noise limit, can be written

$$\rho_{\text{as}}(E)=\xi^{-2}A(E+\xi C_0)\exp[-B(E+\xi C_0)/2\xi], \tag{5.20}$$

where the constant C_0 and the functions A and B are independent of ξ, and only C_0 is sensitive to the short-wavelength cutoff in W. The function B is the same as in Eq. (4.8) for $\rho_1(E)$, but the function A is changed.[14]

6. MOMENTUM-DEPENDENT SPECTRAL DENSITY

The theory of the low-energy tail developed in I and the present paper can be used to discuss the momentum-dependent spectral density $A(\mathbf{k},E)$, as well as the density of states $\rho(E)$. The spectral density is defined by

$$A(\mathbf{k},E)\equiv\frac{1}{\Omega}\langle\sum_i|\Psi_i(\mathbf{k})|^2\delta(E-E_i)\rangle, \tag{6.1}$$

where

$$\Psi_i(\mathbf{k})=\int e^{-i\mathbf{k}\cdot\mathbf{x}}\psi_i(\mathbf{x})d\mathbf{x}. \tag{6.2}$$

Thus $A(\mathbf{k},E)$ equals $\rho(E)$ multiplied by the expectation value of the square of the Fourier transform of the wavefunctions at energy E. The spectral density is normalized so that

$$\frac{1}{(2\pi)^3}\int A(\mathbf{k},E)d\mathbf{k}=\rho(E). \tag{6.3}$$

In the first approximation, the form of the wave functions ψ_i at energy E is given by the function f which maximizes $\rho_f(E)$. We are therefore led to approximation (2.17) of I,

$$A(\mathbf{k},E)\approx|f(\mathbf{k})|^2\rho(E). \tag{6.4}$$

Needless to say, one will obtain a better approximation to the spectral density if one employs in (6.4) the true asymptotic form for the density of states, or the approsimation $\rho_2(E)$, than if one employs the simple approximation $\rho_1(E)$. One may also ask, however, what corrections can one find to the *momentum dependence* of (6.4) by taking into account the difference between $V(\mathbf{x})$ and $V_0(\mathbf{x}-\mathbf{y})$, in the spirit of the present paper. We shall discuss here only the case of a Gaussian random potential.

In order to obtain an improved wave function, we may expand ψ_i in powers of the perturbation $[V(\mathbf{x})-V_0(\mathbf{x}-\mathbf{x}_i)]$. We write

$$\psi_i(\mathbf{x})=f(\mathbf{x}-\mathbf{x}_i)+f_1(\mathbf{x})+f_2(\mathbf{x})+\cdots, \tag{6.5}$$

where

$$f_1(\mathbf{x})=\int\hat{G}(\mathbf{x},\mathbf{x}')f(\mathbf{x}')[V(\mathbf{x}')-V_0(\mathbf{x}'-\mathbf{x}_i)]d\mathbf{x}', \tag{6.6}$$

and similar expressions may be given for f_2, etc. It is clear that in the limit $\xi\rightarrow 0$, the perturbation terms will become relatively unimportant, and thus we must have

$$\lim_{\xi\rightarrow 0}\frac{A(\mathbf{k},E)}{\rho(E)}=|f(\mathbf{k})|^2. \tag{6.7}$$

As mentioned in Sec. 4 of I, relation (6.7) can be directly confirmed, for the one-dimensional Gaussian white-noise case by comparison with the exact theory of Ref. 9.

The first correction terms to (6.7) will be of order ξ, and can be calculated by a method similar to that employed for the complete higher-order energy correction to the density of states of Sec. 5. The calculations are

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[14] [*Note added in proof.* In Eq. (5.16) and subsequent equations, we have assumed that $2\mu\alpha_n<1$, for all $n\geq 4$. It can be shown, as a consequence of the fact that the function f has been chosen to minimize $\Gamma(E,f)$, that $2\mu\alpha_n\leq 1$ for all $n\geq 4$. We have not been able to disprove the possibility that $2\mu\alpha_n=1$, however. If the equality should hold, or almost hold, for some $n\geq 4$, then we must be more careful in deriving the integrand on the right-hand side of (5.16), and must keep terms through η_n^4 in the exponent. The simple result for the correction factor, $\Pi_{n=4}^{\infty}(1-2\mu\alpha_n)^{-1/2}$, appearing in Eqs. (5.16), (5.18), and (5.19), would then be replaced by a somewhat more complicated expression, and would no longer be independent of ξ].

rather complicated, however, and we shall not give details here. In most cases the corrections will be small and not very interesting. There are two situations, however, in which the corrections may be important.

The first case occurs when the second-order energy shift ϵ_2 is large, as for the white-noise limit in two or three dimensions. In that case, to find the spectral density at energy E, one must use in (6.4) not the function f which maximizes $\rho_f(E)$, but the function f which maximizes $\rho_f(E+\xi C_0)$. This correction is consistent with the point of view that the principal effect of the large second-order energy shift is to displace the band as a whole. In other words, the shape f, which we assigned to wave functions at energy E, in the theory of approximation ρ_1, really is appropriate for wave functions with the displaced energy $E-\xi C_0$.

The second situation where (6.4) may be inadequate occurs when one is interested in large values of the wave vector $\mathbf{k}$. It can be shown that the function $f(\mathbf{x})$ is an analytic function of $\mathbf{x}$, and the Fourier transform $f(\mathbf{k})$ must fall off faster than any power of k, as $\mathbf{k}\rightarrow\infty$. On the other hand, if the impurity potentials are nonanalytic at the impurity sites, the expectation value of the absolute square of the Fourier transform of $V(\mathbf{x})$ will fall off as some power of $1/k$. It is clear that the short-wavelength fluctuations in $V(\mathbf{x})$ must produce short-wavelength fluctuations in the wave function by first-order perturbation theory, and the admixture of short-wavelength components will also fall off as some power of $1/k$. In fact, one can show that in the limit $k\rightarrow\infty$, for fixed E and ξ, the spectral density has the form

$$A(\mathbf{k},E)\sim\rho(E)\xi W(\mathbf{k})/[E(\mathbf{k})-E_0]^2. \tag{6.8}$$

In (6.8), $E(\mathbf{k})$ is the energy of the state of wave vector $\mathbf{k}$ in the absence of the random potential $V(\mathbf{x})$, and $W(\mathbf{k})$ is the Fourier transform of $W(\mathbf{x}-\mathbf{x}')$ and is proportional to the absolute square of the Fourier transform of the impurity potentials. For the one-dimensional white-Gaussian-noise model, (6.8) becomes

$$A(k,E)\sim 2\xi k^{-4}\rho(E), \tag{6.9}$$

in agreement with the results of Ref. 9 for the form of the spectral density in the limit of large k.

7. SUMMARY

In I, a variational approximation $E_f(\mathbf{x}_i)$ to the energy eigenvalues E_i was obtained under the approximation that all the eigenstates at a given energy have the same shape, or equivalently, that all the corresponding potential wells have the same shape. Using this variational estimate of the energies, we were led to the approximate density of states ρ_1. In the present paper, we have studied the difference between the exact and variational energies by treating the differences between the actual well shapes and the "typical well shape" as small perturbations. We have proposed an approximate density of states $\rho_2(E)$ in which all the energies $E_f(\mathbf{x}_i)$ are displaced by the average of the difference between E_i and $E_f(\mathbf{x}_2)$. Although calculation of ρ_2 is difficult in general, it is feasible in the limit of a Gaussian random potential (infinite density of weak impurities). The Gaussian case is relatively simple because in this case, only the second-order perturbation correction is important, and because the necessary calculations of conditional correlation functions of the random potential are easy to perform.

It is in fact possible to calculate the asymptotic form of the exact density of states, for the Gaussian case, by a slight generalization of the work of Zittartz and Langer, although such a calculation is more difficult than the calculation of ρ_2. When the energy corrections are small, the density of states in a three-dimensional Gaussian potential has the form

$$\rho(E)=\xi^{-2}A(E)\exp[-B(E)/2\xi], \tag{7.1}$$

where ξ is a parameter proportional to the concentration of impurities and to the square of the strengths of the individual impurities, and where A and B are functions of the energy E and, implicitly, of the *shapes* of the impurity potentials. The parameter ξ is proportional to the variance of the potential fluctuations, and in the low-energy tail it is small relative to the value of $B(E)$.

The function B in (7.1) is the same for the true asymptotic form of ρ as for the approximations $\rho_2(E)$ and $\rho_1(E)$; the function A is different in each case. In the white-noise limit in two or three dimensions, a large second-order energy correction is found, and (7.1) must be modified.

The spectral density $A(\mathbf{k},E)$ has a momentum dependence which is approximately given by

$$A(\mathbf{k},E)=|f(\mathbf{k})|^2\rho(E), \tag{7.2}$$

where $f(\mathbf{k})$ is the Fourier transform of the shape of the "typical wave function" at energy E, found in I. In the low-energy tail, for a Gaussian potential, corrections to (7.2) are small except in the case of large wave vector $\mathbf{k}$, or in the case of a large second-order energy correction.

APPENDIX: EVALUATION OF SECOND-ORDER ENERGY-SHIFT INTEGRAL IN THE ONE-DIMENSIONAL CASE

Before evaluating the necessary integral (4.16), we note that for the one-dimensional white-Gaussian-noise model, $f(x)$ scales as $(\kappa)^{1/2}$, i.e.,

$$f(x)=\kappa^{1/2}g(\kappa x), \tag{A1}$$

where g is a function independent of the energy. In the same sense, $\hat{G}\propto\kappa^{-1}$, $w(x,x')\propto\kappa$, and $dx=\kappa^{-1}d(\kappa x)$ so that using (4.16)

$$C(E)=c/\kappa, \tag{A2}$$

where c is a constant independent of κ. In view of (4.20) and $\mu=4\kappa$ [see I, Eq. (B10)],

$$\rho_2(E)=e^{\mu c/\kappa}\rho_1(E)=e^{4c}\rho_1(E)\,, \tag{A3}$$

where the parameter c can be evaluated using (4.16) at $\kappa=1$, i.e., $c=C(E=-\frac{1}{2})=C(\kappa=1)$ or

$$-c=\int f(x)\hat{G}(x,x')f(x')w(x',x)dxdx'\,, \tag{A4}$$

where all functions in the integrand of (A4) are to be evaluated with $\kappa=1$. Using (4.23), (4.28), and (4.29), we have

$$f(x)=(1/2)^{1/2}\,\mathrm{sech}x\,, \tag{A5}$$

$$\hat{G}(x,x')=f(x)f(x')H(x,x')\,, \tag{A6}$$

where

$$\begin{aligned} H(x,x')&=x'-x-\tfrac{1}{2}e^{2x}-\tfrac{1}{2}e^{-2x'}, \quad x'\geq x\,,\\ &=x-x'-\tfrac{1}{2}e^{2x'}-\tfrac{1}{2}e^{-2x}, \quad x'\leq x\,, \end{aligned} \tag{A7}$$

$$\begin{aligned} w(x,x')&=\tfrac{1}{2}\delta(x-x')-(3/2)f^2(x)f^2(x')\,,\\ &-(15/2)f(x)[df(x)/dx]f(x')[df(x')/dx']. \end{aligned} \tag{A8}$$

Using (A8) and $H(x,x')=H(x',x)$, we can split (A4) into three terms:

$$-c=I_1+I_2+I_3\,, \tag{A9}$$

$$I_1=\frac{1}{2}\int_{-\infty}^{\infty} dx\, f^4(x)H(x,x)\,, \tag{A10}$$

$$I_2=-3\int_{-\infty}^{\infty} dx\int_x^{\infty} dx'\, f^4(x)f^4(x')H(x,x')\,, \tag{A11}$$

$$I_3=-\frac{15}{16}\int_{-\infty}^{\infty} df^4(x)\int_x^{\infty} H(x,x')df^4(x')\,, \tag{A12}$$

where, from now on, $H(x,x')$ stands for the first form in (A7).

Introducing $u=\exp(-2x)$, we evaluate I_1:

$$I_1=-\int_{-\infty}^{\infty} dx\frac{e^{2x}+e^{-2x}}{(e^x+e^{-x})^4}=-\frac{1}{2}\int_0^{\infty}\frac{u^2+1}{(1+u)^4}du=-\tfrac{1}{3}. \tag{A13}$$

A direct evaluation of I_3 leads to many terms. Integration by parts on x', however, simplifies I_3 to

$$I_3=-\frac{15}{16}\int_{-\infty}^{\infty} df^4(x)\Big[f^4(x)\cosh 2x -\int_x^{\infty} f^4(x')(1+e^{-2x'})dx'\Big]. \tag{A14}$$

But $f^3(x)df(x)/dx$ is an odd function of x, so the first term in (A14) yields a vanishing contribution. Integrating by parts now on x, and dropping the vanishing boundary term,

$$I_3=\frac{15}{16}\int_{-\infty}^{\infty} f^8(x)(1+e^{-2x})dx. \tag{A15}$$

But the even part of $1+e^{-2x}$ is

$$\tfrac{1}{2}[(1+e^{-2x})+(1+e^{2x})]=2\cosh^2 x\,,$$

so that in view of (A5)

$$I_3=\frac{(15)\times 2}{(16)^2}\int_{-\infty}^{\infty}\mathrm{sech}^6 x dx. \tag{A16}$$

The integral in (A16) can be evaluated by changing variables to $u=\exp(-2x)$:

$$I_3=\frac{15}{4}\int_0^{\infty}\frac{u^2du}{(1+u)^6}=\tfrac{1}{8}. \tag{A17}$$

Using $u=\exp(-2x)$, $u'=\exp(-2x')$, $f^2(x)=2u/(1+u)^2$, we can rewrite I_2 in the form

$$I_2=-3\int_0^{\infty}\frac{udu}{(1+u)^4}\Big[\Big(\ln u-\frac{1}{u}\Big)\int_0^u\frac{2u'du'}{(1+u')^4} -\int_0^u\frac{2(u'+\ln u')}{(1+u')^4}u'du'\Big] \tag{A18}$$

or

$$\begin{aligned} I_2=-3\int_0^{\infty}\frac{udu}{(1+u)^4}\Big\{&\Big(\ln u-\frac{1}{u}\Big)\Big[\frac{1}{3}-\frac{1}{(1+u)^2}+\frac{2}{3}\frac{1}{(1+u)^3}\Big]\\ &-\Big[\frac{2}{3}-\frac{2}{1+u}+\frac{2}{(1+u)^2}-\frac{2}{3}\frac{1}{(1+u)^3}\Big]\\ &+2[F_3(u)-F_4(u)]-2[F_3(0)-F_4(0)]\Big\}\,, \end{aligned} \tag{A19}$$

where

$$\begin{aligned} F_n(u)&=\int_u^{\infty}\frac{\ln v}{(1+v)^n}dv\\ &=\frac{1}{n-1}\frac{\ln u}{(1+u)^{n-1}}+\frac{1}{n-1}\int_u^{\infty}\frac{dv}{v(1+v)^{n-1}}, \end{aligned} \tag{A20}$$

after an integration by parts. Introducing the partial fraction expansion

$$\frac{1}{v(1+v)^{n-1}}=\frac{1}{v}-\sum_{m=1}^{n-1}\frac{1}{(1+v)^m}, \tag{A21}$$

we obtain

$$F_n(u)=\frac{\ln u}{(n-1)(1+u)^{n-1}}+\frac{1}{n-1}\Big[\ln\frac{1+u}{u} -\sum_{s=1}^{n-2}\frac{1}{s}\frac{1}{(1+u)^s}\Big], \tag{A22}$$

$$F_n(0)=-\frac{1}{n-1}\Big[1+\tfrac{1}{2}+\tfrac{1}{3}+\cdots+\frac{1}{n-2}\Big]. \tag{A23}$$

Inserting these results into (A19), we find that all terms proportional to $\ln u$ fortuitously cancel. After a rearrangement, we get

$$I_2=-6\int_0^\infty du\left[-\frac{1}{3}\frac{1}{(1+u)^3}+\frac{1}{(1+u)^4}-\frac{5}{3}\frac{1}{(1+u)^5}+\frac{5}{3}\frac{1}{(1+u)^6}-\frac{2}{3}\frac{1}{(1+u)^7}+\frac{1}{6}\frac{\ln(1+u)}{(1+u)^3}-\frac{1}{6}\frac{\ln(1+u)}{(1+u)^4}\right], \tag{A24}$$

$$I_2=-6\left[-\frac{1}{6}+\frac{1}{3}-\frac{5}{12}+\frac{1}{3}-\frac{1}{9}+\frac{1}{24}-\frac{1}{54}\right]=\frac{1}{36}, \tag{A25}$$

$$c=-(I_1+I_2+I_3)=-\left(-\frac{1}{3}+\frac{1}{36}+\frac{1}{8}\right)=\frac{13}{72}. \tag{A26}$$

In view of (A2), we thus obtain the result (4.30) for $C(E)$ and the correction factor

$$\exp[\mu C(E)]=\exp(13/18), \tag{A27}$$

of (4.31), to the density of states.

The average-second-order energy correction can also be evaluated directly from Eq. (5.17), if one uses the results of Zittartz and Langer for the eigenvalues α_n. From Eq. (6.13) of ZL we find

$$\mu\alpha_n=2/[n(n+3)]. \tag{A28}$$

In the one-dimensional case, the sum in (5.17) must run from $n=2$ to ∞. Hence we find

$$\mu C(E)=\sum_{n=2}^{\infty}\mu\alpha_n=\tfrac{2}{3}\sum_{n=2}^{\infty}\left[\frac{1}{n}-\frac{1}{n+3}\right]$$
$$=\frac{2}{3}\left[\frac{1}{2}+\frac{1}{3}+\frac{1}{4}\right]=\frac{13}{18}.$$

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Infrared Studies of Defect Production in *n*-Type Si: Irradiation-Temperature Dependence*

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Infrared absorption measurements of electron-irradiated oxygen-doped *n*-type silicon are presented. The silicon samples were electron irradiated at carefully controlled irradiation temperatures between 75°K and room temperature. Since the free Si vacancy, and presumably also the free Si interstitial, are mobile at these temperatures, intensity measurements of the vacancy-oxygen center, as well as of newly observed infrared absorption bands, provide a monitor of the intrinsic defect production. For irradiation temperatures below 100°K, semilog plots of the intensities of the absorption bands for identical samples versus the reciprocals of their irradiation temperatures yield straight lines having the form $\alpha=\text{const}\ e^{-\Delta E/kT}$. On the basis of the slopes and intensities of these lines, the absorption bands can be divided into two groups. The more intense group, which includes the 836-cm^{-1} (A-center) band and bands at 922, 932, and 865 cm^{-1}, has a common energy $\Delta E=0.05\pm0.005$ eV. Less intense bands at 936, 945, and 956 cm^{-1} are found to have a common energy $\Delta E'=0.10\pm0.02$ eV. These results are interpreted on the basis of a metastable interstitial-vacancy pair model in which the irradiation-temperature dependence of the formation of the defect-impurity complexes results from the temperature dependence of the production of intrinsic defects. On the basis of this model, the difference in the barriers to liberation and recombination of the metastable pair is 0.05 eV for *n*-type Si. The more intense infrared bands are concluded to be associated with complexes composed of a single vacancy or a single interstitial trapped at an oxygen impurity atom or group of atoms. Since the energies $\Delta E'$ of the weaker infrared absorption bands are approximately twice those for the strong infrared bands, it is suggested that the weaker bands are associated with complexes composed of two intrinsic defects trapped at an oxygen impurity center.

I. INTRODUCTION

Electron-paramagnetic-resonance (EPR) measurements by Watkins *et al.*[1] on the production of the vacancy-oxygen (A) center in *n*-type Si have shown that electron irradiations at 20°K or at 77°K with subsequent warming to room temperature produce only a few percent of the defects formed by an equivalent room-temperature irradiation. The same effect was observed by Wertheim[2] for electrical measurements of electron-irradiated *n*-type Si. Wertheim[2] proposed a metastable pair model to explain the irradiation-temperature dependence of the introduction rate, but a detailed

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