

Green's Functions for a Particle in a One-Dimensional Random Potential*

BERTRAND I. HALPERIN†‡

University of California, Berkeley, California

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A method has been found for exactly calculating the spectral density $A(k, E)$ for a particle in a one-dimensional random potential, when the potential at each point is statistically independent of the potential at all other points. Generalizations of this method can also be used to find the phonon Green's functions for a chain of atoms of random mass, or to find various two-particle functions, such as the electrical conductivity of a system of noninteracting electrons in a random potential. Two functions of the position x on the line are defined, which depend on the particular potential configuration and on the parameters k and E . The spectral density is expressed in terms of the probability distribution of these functions when x is at the right-hand end of the line. The distribution is known at the left-hand end, and the values of the functions, as x moves from left to right, form a Markoff process. One can therefore obtain the spectral density by solving the equation of motion for the probability distribution. Further simplification is possible because it is sufficient to know the first two moments of the joint distribution with respect to one variable, and because in the limit of an infinite line, only the asymptotic form of these moments is necessary. The spectral density requires the solution of a pair of differential or integral equations in one variable, while two-particle functions involve similar equations in two variables. Calculations have been carried out for the spectral density of a Schrödinger particle in a "white-Gaussian-noise" potential and of a particle confined to fixed lattice sites in a random thermal-deformation potential.

INTRODUCTION

MANY problems which are difficult or impossible to solve in three dimensions turn out to be readily solvable in one dimension. One class of problems which has been studied successfully in one dimension is the calculation of the density of energy eigenstates of a particle moving in a potential which is not known exactly, but which obeys a statistical distribution such that the potential at one point is independent of the potential at all other points.¹⁻⁴ Another closely related problem which has been solved is the density of normal modes as a function of frequency for a chain of several kinds of atoms occurring in random order.^{2,5,6} For many purposes, however, one is interested not in the density of states, but in a more complicated function, such as the spectral density associated with a state of a given wave vector, or in two-particle Green's functions of various kinds. In the present paper, a method is presented for exact solution of one-dimensional models for a number of these problems.

The single-particle spectral density $A(k, E)$ is of particular interest when the particle is an exciton in a lattice distorted by thermal fluctuations. Under proper circumstances, the line shape for the optical absorption due to an exciton in a nondegenerate band is given by the spectral density of the zero-momentum exciton state.^{7,8}

For *electrons* in an imperfect lattice, the one-particle Green's function is of less direct interest, but it is still useful for understanding the nature of the energy eigenstates. A slightly generalized form of $A(k, E)$ for the phonon modes of a disordered lattice is of interest for the inelastic scattering of neutrons and for infrared absorption by the lattice. Among the problems which require knowledge of two-particle Green's functions are the conductivity of electrons in an imperfect lattice and the optical absorption due to interband transitions in a nonmetal. The methods of the present paper are restricted to cases of noninteracting particles.

The essential features of the methods of this paper are as follows: We consider the problem of finding the spectral density $A(k, E)$ for a particle in a random potential on the line segment $0 \leq x \leq L$. One first defines certain mathematical quantities z and U_1 , which are functions of the position x on the line, as well as of k and E , and of the particular potential configuration. The spectral density may be written as an average, over the potential configurations in the ensemble, of a certain function of the values of z and U_1 at the position $x=L$; hence $A(k, E)$ is determined by the probability distribution of the values of z and U_1 at the right-hand end of the line. The functions z and U_1 are defined in such a way that for $x=0$ they are independent of the potential configuration, and at any other position x , they depend only on the potential to the left of x . Furthermore, they depend on the potential in such a way that if the potential has the property that its value at each point on the line is independent of the value at all other points, then the values of z and U_1 constitute a Markoff process as x goes from 0 to L . Consequently, one can write down an "equation of motion" for the joint probability distribution of z and U_1 , which one must then integrate from $x=0$ to $x=L$ in order to find the distribution at $x=L$. An important mathematical simplification is possible

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† Present address: Princeton University, Princeton, New Jersey.

‡ National Science Foundation Graduate Fellow.

¹ H. L. Frisch and S. P. Lloyd, *Phys. Rev.* **120**, 1175 (1960).

² H. Schmidt, *Phys. Rev.* **105**, 425 (1957).

³ M. Lax and J. C. Phillips, *Phys. Rev.* **110**, 41 (1958).

⁴ R. E. Borland, *Proc. Phys. Soc. (London)* **77**, 705 (1961).

⁵ F. J. Dyson, *Phys. Rev.* **92**, 1331 (1953).

⁶ R. L. Agacy, *Proc. Phys. Soc. (London)* **83**, 581 (1964); R. E. Borland, *Proc. Phys. Soc. (London)* **83**, 1027 (1964).

⁷ J. J. Hopfield, *J. Phys. Chem. Solids* **22**, 63 (1961).

⁸ Y. Toyozawa, *Progr. Theoret. Phys. (Kyoto)* **20**, 53 (1958).

because the nature of the equation of motion enables one to work with the zeroth, first, and second moments with respect to U_1 of the joint distribution, for each value of z , rather than the distribution itself. When one is interested in the case of very large L , it is only necessary to find the asymptotic form, for large x , of these moments, and further simplification results.

The calculation of two-particle functions is similar in principle to the calculation of $A(k, E)$, but the variable z is replaced by two variables, z and z' .

In Sec. 1, $A(k, E)$ is found for a Schrödinger particle in a potential whose fluctuations, as a function of position, may be described as "white Gaussian noise." Such a potential can arise as the potential due to a random array of point scatterers in the limit of infinite density of scatterers, or as a deformation potential due to thermal fluctuations of a continuous, classical, harmonic elastic string. The particle may be an electron or an exciton in the effective-mass approximation. The total density of states for this model can be found by the method of Frisch and Lloyd,¹ and as shown in Appendix B of the present paper, can be expressed analytically in terms of Airy functions. The spectral density $A(k, E)$ is expressed, for each value of k and E , in terms of the solution of an ordinary differential equation, and has been computed numerically for several values of k and a range of values of E . The exact values of the spectral density are compared with the results of a self-consistent Green's-function approximation in which one sums a selected set of diagrams in the perturbation series. The asymptotic forms for $A(k, E)$ are found analytically for fixed k , with $E \rightarrow \pm \infty$, and for fixed E , with $k \rightarrow \infty$. At the end of Sec. 1, the generalization of the procedure for finding $A(k, E)$ to handle Schrödinger particles in other random potentials is briefly discussed.

In Sec. 2, we discuss applications of the method to a model of an exciton or an electron in an energy band of finite width, in a lattice perturbed by thermal fluctuations. Here the position of the particle is restricted to a discrete set of lattice sites, and the Hamiltonian has terms which connect nearest-neighbor sites, as well as terms diagonal in the position of the particle. The spectral density for the problem is given in terms of the solutions of a pair of integral equations in one variable. These have been solved numerically for several values of the parameters involved and have been plotted to show the transition from the case of infinite bandwidth (Sec. 1) to the case of zero bandwidth.

In Sec. 3, we discuss the phonon spectral density for a chain of random mass, with a harmonic interaction between nearest neighbors. The equations derived are similar to those of Sec. 2.

Finally, in Sec. 4, we illustrate applications to two-particle Green's functions by deriving the equations for the frequency-dependent conductivity of a system of noninteracting electrons in the white-Gaussian-noise potential of Sec. 1, and by briefly discussing a model for

interband optical transitions in a nonmetal. The two-particle functions are expressed in terms of a pair of partial differential equations in two variables. No numerical examples have been calculated for Secs. 3 and 4.

1. SCHRÖDINGER PARTICLES

White-Gaussian-Noise Potential

We wish to find the spectral density for a particle on the line segment $0 \leq x \leq L$ obeying the Hamiltonian

$$H = (-\hbar^2/2m^*)(d^2/dx^2) + V(x), \quad (1.1)$$

where V is a random potential described by a Gaussian statistical distribution with the expectation values

$$\langle V(x) \rangle = 0, \quad (1.2)$$

$$\langle V(x)V(x') \rangle = \frac{1}{2}D\delta(x-x'), \quad (1.3)$$

where D is a constant and δ is the Dirac δ function. The wave functions are assumed to satisfy boundary conditions of the form

$$\psi'(0) = z_0\psi(0), \quad (1.4)$$

$$\psi'(L) = z_L\psi(L), \quad (1.5)$$

where z_0 and z_L are arbitrary real constants.

The potential V is described as white Gaussian noise, because its Fourier amplitudes have a Gaussian distribution with standard deviations independent of the frequency, and with no correlations between the amplitudes at different frequencies. Because a Gaussian distribution of any number of variables is completely described by its first and second moments, Eq. (1.3) implies that the potential at any point is completely independent of the potentials at all other points.

The white-Gaussian-noise potential may arise from a deformation potential on an infinitely massive continuous string. Let the deformation potential be given by

$$V(x) = V_0 dR(x)/dx, \quad (1.6)$$

where $R(x)$ is the displacement from equilibrium of the point x on the string. We assume that the string obeys Hooke's law exactly with elastic modulus B . Then, according to classical statistical mechanics, the potential V has a Gaussian-white-noise distribution with the constant D given, at temperature T , by

$$D = 2V_0^2 k_B T / B, \quad (1.7)$$

where k_B is Boltzmann's constant.

An alternate interpretation of V is the potential arising, in the high-density limit, from the model used by Frisch and Lloyd¹ for an impurity band—a set of δ -function potentials of fixed magnitude, distributed at random on the line. In the high-density limit, the fluctuations about the average potential have a Gaussian-white-noise distribution with

$$D = 2nv_0^2, \quad (1.8)$$

where v_0 is the coefficient of the δ -function potential and n is the number of scatterers per unit length.

The spectral density for a one-dimensional Schrödinger particle in a random potential is defined by

$$A(k, E) \equiv \frac{1}{L} \left\langle \sum_i \left| \int_0^L e^{ikx} \psi_i(x) dx \right|^2 \delta(E - E_i) \right\rangle, \quad (1.9)$$

where E_i and ψ_i are the energy and wave function of the i th eigenstate of the Hamiltonian. (Throughout this paper we use angular brackets $\langle \dots \rangle$ to indicate an average over the statistical ensemble.) The total density of states at energy E is defined by

$$\rho(E) = L^{-1} \langle \sum_i \delta(E - E_i) \rangle. \quad (1.10)$$

The spectral density is normalized so that

$$\int_{-\infty}^{\infty} A(k, E) dE = 1, \quad (1.11)$$

$$(2\pi)^{-1} \int_{-\infty}^{\infty} A(k, E) dk = \rho(E). \quad (1.12)$$

The spectral density is equal to $-1/\pi$ times the imaginary part of the Green's function $G(k, E)$ for the particle at energy E and wave vector k .⁹

In the problem we are considering, it is always possible to choose units of length, time, and mass, such that $\hbar = m^* = D = 1$; in the remainder of this section, we shall assume this has been done. To obtain results in any other system of units, it is necessary to substitute for E , in the expressions given below, the energy divided by the unit of energy, $\epsilon_0 = (D^2 m^* \hbar^{-2})^{1/3}$, and to substitute for k and L^{-1} the wave vector and inverse crystal size divided by the unit of reciprocal length, $\kappa_0 = (D m^* \hbar^{-4})^{1/3}$. In addition, the expressions for the spectral density must be multiplied by the over-all factor ϵ_0^{-1} , while the total density of states must be multiplied by $\epsilon_0^{-1} \kappa_0$.

Procedure

For each potential configuration in the ensemble of possible configurations, we define the function $\varphi(x; E)$ to be the unique solution of the second-order differential equation

$$-\frac{1}{2}(\partial^2/\partial x^2)\varphi + V(x)\varphi = E\varphi, \quad (1.13)$$

with the initial conditions

$$\varphi(0; E) = 1, \quad (1.14)$$

$$(\partial\varphi/\partial x)(0; E) = z_0\varphi(0; E). \quad (1.15)$$

Note that although φ obeys the Schrödinger equation for energy E , it will not be an energy eigenstate unless it also obeys the boundary condition $(\partial\varphi/\partial x)(L; E) = z_L\varphi(L; E)$. Furthermore, φ will not, in general, be

⁹ D. Pines, *The Many-Body Problem* (W. A. Benjamin, Inc., New York, 1961), p. 31.

properly normalized on the interval $0 \leq x \leq L$. We also define the four functions

$$z(x; E) \equiv [\partial\varphi(x; E)/\partial x]/\varphi(x; E), \quad (1.16)$$

$$U_1(x; E) \equiv \left[\int_0^x e^{ikx'} \varphi(x'; E) dx' \right] / e^{ikx} \varphi(x; E), \quad (1.17)$$

$$U_2(x; E) \equiv \left[\int_0^x \varphi(x'; E)^2 dx' \right] / \varphi(x; E)^2, \quad (1.18)$$

$$U_3(x; E) \equiv \partial z(x; E)/\partial E. \quad (1.19)$$

From (1.16) and (1.13), we find that $z(x; E)$ obeys the "equation of motion"

$$\frac{\partial z}{\partial x} = \left[\frac{\partial^2 \varphi}{\partial x^2} - \left(\frac{\partial \varphi}{\partial x} \right)^2 \right] / \varphi^2 = -z^2 - 2E + 2V(x). \quad (1.20)$$

Similarly, U_1 and U_2 obey

$$\partial U_1/\partial x = 1 - zU_1 - ikU_1, \quad (1.21)$$

$$\partial U_2/\partial x = 1 - 2zU_2. \quad (1.22)$$

Differentiating both sides of Eq. (1.20) with respect to E , we find

$$\partial U_3/\partial x = -2 - 2zU_3. \quad (1.23)$$

At $x=0$, we have the initial conditions $z=z_0$ and $U_1=U_2=U_3=0$. If x_n is a point such that $\varphi(x_n; E)=0$, then the quantities z , U_1 , U_2 , and U_3 all become infinite at $x=x_n$. However, the four quantities $(x-x_n)z$, $(x-x_n)U_1$, $(x-x_n)^2U_2$, and $(x-x_n)^2U_3$ are continuous in the neighborhood of x_n . With these conditions, the four differential equations (1.20)–(1.23) uniquely determine z , U_1 , U_2 , and U_3 for all x . Comparison of equations (1.22) and (1.23) establishes that, for all x ,

$$U_3(x; E) = -2U_2(x; E). \quad (1.24)$$

Since U_2 is greater than zero, for $x>0$, it follows that U_3 is less than zero.

For each potential configuration, the energy E_i of the i th eigenstate is the i th value of E which satisfies the equation $z(L; E) = z_L$. Hence,

$$\sum_i \delta(E - E_i) = \delta[z_L - z(L; E)] |\partial z(L; E)/\partial E|. \quad (1.25)$$

It follows that

$$\begin{aligned} A(k, E) &= \frac{1}{L} \left\langle \frac{|\int_0^L \varphi(x; E) e^{ikx} dx|^2}{\int_0^L \varphi(x; E)^2 dx} \sum_i \delta(E - E_i) \right\rangle, \\ &= \frac{1}{L} \left\langle \frac{|U_1(L; E)|^2}{U_2(L; E)} |U_3(L; E)| \delta[z_L - z(L; E)] \right\rangle, \\ &= 2L^{-1} \langle |U_1(L; E)|^2 \delta[z - z(L; E)] \rangle. \end{aligned} \quad (1.26)$$

Let us restrict ourselves, temporarily, to the case of $k=0$, in order to avoid complications due to the presence

of complex numbers. The joint probability distribution of z and U_1 , at the point x , is defined by

$$P(z, U_1; x) \equiv \langle \delta[z - z(x; E)] \delta[U_1 - U_1(x; E)] \rangle. \quad (1.27)$$

The spectral density is given by

$$A(0, E) = 2L^{-1} \int_{-\infty}^{\infty} U_1^2 P(z_L, U_1; L) dU_1. \quad (1.28)$$

The spectral density would be determined, if one knew the probability distribution of z and U_1 at $x=L$. The distribution at $x=0$ is known:

$$P(z, U_1; 0) = \delta(z - z_0) \delta(U_1). \quad (1.29)$$

If we can find and solve an "equation of motion" for the probability distribution, as x moves from left to right on the line, we will be able to obtain the spectral density. If the potential $V(x)$ were absent in Eq. (1.20) the probability distribution would obey the simple "flow" equation

$$\begin{aligned} \frac{\partial P}{\partial x} &= -\frac{\partial}{\partial z} \left(\frac{\partial z}{\partial x} P \right) - \frac{\partial}{\partial U_1} \left(\frac{\partial U_1}{\partial x} P \right) \\ &= \left[\frac{\partial}{\partial z} (z^2 + 2E) + \frac{\partial}{\partial U_1} (zU_1 - 1) \right] P. \end{aligned}$$

The random potential $V(x)$ causes a "random walk" of the quantity z , with $\langle [z(x+dx; E) - z(x; E)]^2 \rangle = 2dx$. This adds a diffusion term $\partial^2 P / \partial z^2$ to the equation of motion:

$$\frac{\partial P}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} (z^2 + 2E) + \frac{\partial}{\partial U_1} (zU_1 - 1) \right] P. \quad (1.30)$$

Equation (1.30) has precisely the form of the Fokker-Planck equation, and is exact when $V(x)$ has the form of white Gaussian noise.¹⁰

The distribution of z and U_1 obeys boundary conditions at infinity which are determined by the behavior of z and U_1 at the zeros of φ . Together with these boundary conditions, Eqs. (1.29) and (1.30) determine $P(z, U_1; x)$ for all x . The solution of a partial differential equation such as (1.30) involves formidable numerical computations, however, and it is fortunate that several simplifications can be made. We define the three functions $P_s(z; x)$, ($s=0, 1, 2$), by

$$\begin{aligned} P_s(z; x) &\equiv \langle U_1(x; E)^s \delta[z - z(x; E)] \rangle \\ &= \int_{-\infty}^{\infty} P(z, U_1; x) U_1^s dU_1. \end{aligned} \quad (1.31)$$

The function $P_0(z; x)$ is just the probability distribution of $z(x; E)$, while P_1 and P_2 are the first and second mo-

¹⁰ For a derivation of the Fokker-Planck equation, see M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. 17, 323 (1945).

ments with respect to U_1 of the joint distribution of z and U_1 . These functions obey the equations of motion

$$\frac{\partial P_0}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} (z^2 + 2E) \right] P_0, \quad (1.32)$$

$$\frac{\partial P_1}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} (z^2 + 2E) - z \right] P_1 + P_0, \quad (1.33)$$

$$\frac{\partial P_2}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + (z^2 + 2E) \frac{\partial}{\partial z} \right] P_2 + 2P_1, \quad (1.34)$$

with the boundary conditions

$$\lim_{z \rightarrow +\infty} z^{2-s} P_s = \lim_{z \rightarrow -\infty} z^{2-s} P_s. \quad (1.35)$$

Equation (1.35) is derived from the properties of z and U_1 at the nodes of φ , where z crosses from $-\infty$ to ∞ .

At the point $x=0$, we have

$$P_0(z; 0) = \delta(z - z_0), \quad (1.36)$$

$$P_1(z; 0) = P_2(z; 0) = 0. \quad (1.37)$$

The differential equations (1.32)–(1.34), together with the boundary conditions, determine P_s , for all x , and are much easier to solve numerically than the equation of motion for $P(z, U_1; x)$. The spectral density is given by

$$A(k, E) = 2L^{-1} P_2(z_L; L). \quad (1.38)$$

When k does not equal zero, certain changes must be made. The definition of P_2 must be modified to

$$P_2(z; x) = \langle |U_1(x; E)|^2 \delta[z - z(x; E)] \rangle. \quad (1.39)$$

Equations (1.33) and (1.34) are replaced by

$$\frac{\partial P_1}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} (z^2 + 2E) - z - ik \right] P_1 + P_0, \quad (1.40)$$

$$\frac{\partial P_2}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + (z^2 + 2E) \frac{\partial}{\partial z} \right] P_2 + 2 \operatorname{Re} P_1. \quad (1.41)$$

The rest of equations (1.31)–(1.38) still apply.

If we are interested in the properties of macroscopic systems, we only need to find the spectral density in the limit $L \rightarrow \infty$; this makes still further simplification possible. In Appendix A, we give physical arguments to show that for large x , the P_s have asymptotic forms

$$P_0(z; x) \sim p_0(z), \quad (1.42)$$

$$P_1(z; x) \sim p_1(z), \quad (1.43)$$

$$P_2(z; x) \sim Cx + f(z), \quad (1.44)$$

where p_0 , p_1 , f , and the constant C are independent of x . The spectral density is given, for large L , by

$$A(k, E) = 2C. \quad (1.45)$$

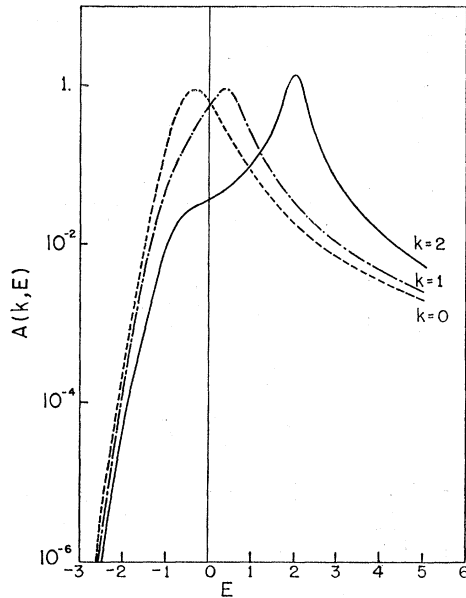


FIG. 1. Spectral density $A(k, E)$ for white-Gaussian-noise potential. Energy is measured in units of $\epsilon_0 = (D^2 m^2 \hbar^{-2})^{1/3}$, wave number in units of $\kappa_0 = (D m^2 \hbar^{-4})^{1/3}$. The spectral density is normalized so that the area under the curve is 1.

It is independent of the length L and independent of the boundary conditions z_0 and z_L imposed on the particle wave functions.

The functions p_0 and p_1 obey Eqs. (1.32) and (1.40), respectively, with the left-hand sides set equal to zero:

$$\left[\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} (z^2 + 2E) \right] p_0 = 0, \quad (1.46)$$

$$\left[\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} (z^2 + 2E) - z - ik \right] p_1 + p_0 = 0. \quad (1.47)$$

The boundary conditions of (1.35) still apply, and p_0 satisfies the normalization

$$\int_{-\infty}^{\infty} p_0(z) dz = 1, \quad (1.48)$$

which is imposed by the fact that $P_0(z; x)$ is a probability distribution. If one substitutes (1.43) and (1.44) in Eq. (1.41), multiplies both sides of the equation by $p_0(-z)$, and integrates with respect to z , one obtains

$$A(k, E) = 4 \int_{-\infty}^{\infty} p_0(-z) \text{Re} p_1(z) dz. \quad (1.49)$$

The simple form of (1.49) arises from the fact that the differential operator on the right-hand side of (1.46) is the adjoint, except for a change of the sign of z , of the operator on the right-hand side of (1.41).

Numerical Calculations

Equations (1.46)–(1.49) reduce the problem of finding the spectral density to the solution of two ordinary differential equations and one numerical quadrature, tasks which are easily handled by an electronic computer. The results of numerical computations of $A(k, E)$ are plotted, for several values of k , in Fig. 1. In Fig. 2, the values of $A(k, E)$ are compared with the approximate values obtained by the “ $\Gamma=1$ approximation” of Suna,¹¹ or equivalently, by “approximation number 3” of Klauder.¹² These are self-consistent Green’s function approximations, which, in effect, sum an infinite set of Feynman diagrams in the perturbation theory expansion of the Green’s function $G(k, E)$, as indicated in Fig. 3. The resulting equations for G are

$$G(k, E) = [E - \frac{1}{2}k^2 - \Sigma(E)]^{-1}, \quad (1.50)$$

$$\Sigma(E) = -2^{-3/2} [\Sigma(E) - E]^{-1/2}. \quad (1.51)$$

The approximate method, as expected, gives good agreement with the exact results for positive energies, but is not very accurate for negative energies. The low-energy tail of the spectral density is entirely absent, in the self-consistent approximation, as (1.51) leads to Green’s functions which are real at energies less than $-\frac{3}{4}\sqrt{2}$ (≈ -0.9449).

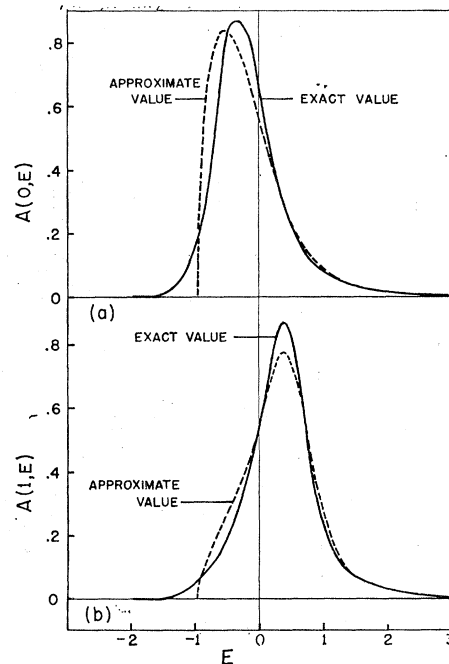


FIG. 2. Comparison of exact values of $A(k, E)$ with results of self-consistent Green’s function approximation, for white-Gaussian-noise potential. (a) Wave number $k=0$. (b) Wave number $k=1$. On this scale, the exact and approximate curves for the spectral density would be almost indistinguishable for $k=2$. Units are the same as in Fig. 1.

¹¹ A. Suna, Phys. Rev. **135**, A111 (1964).

¹² J. R. Klauder, Ann. Phys. (N.Y.) **14**, 43 (1961).

Density of States

The total density of states $\rho(E)$ is somewhat easier to find than $A(k, E)$; for an infinite line, it may be found directly from the function $p_0(z)$. By using the fact that the number of energy eigenstates with energy less than E , in any particular potential configuration, is equal to the number of nodes in the function $\varphi(x; E)$, within a possible error of ± 1 , Frisch and Lloyd¹ show that

$$\lim_{z \rightarrow \pm\infty} z^2 p_0(z) = N(E), \quad (1.52)$$

where $N(E)$ is the cumulative density of states defined by

$$N(E) \equiv \int_{-\infty}^E \rho(E') dE'. \quad (1.53)$$

The function $\rho(E)$ is obtained from $N(E)$ by differentiation. A plot of $N(E)$ for a white-Gaussian-noise potential may be found in Ref. 1, Fig. 6.

The function $\rho(E)$ can also be expressed in terms of the function $p_0(z)$ at the single energy E , by use of the methods of the present paper. It is easily seen that

$$\rho(E) = L^{-1} \langle |U_3(L; E)| \delta[z_L - z(L; E)] \rangle. \quad (1.54)$$

If one studies the equation of motion for the function $\langle U_3(x; E) \delta[z - z(x; E)] \rangle$ in the same manner that we studied the equation of motion for $P_2(z; x)$, one finds that, for large L ,

$$\rho(E) = 2 \int_{-\infty}^{\infty} p_0(-z) p_0(z) dz. \quad (1.55)$$

Analytic Results

It is interesting to see what properties of the eigenstates of the Gaussian-white-noise potential can be derived analytically from Eqs. (1.46)–(1.49). The general solution of the differential equation (1.46) can be written in integral form. The solution which is bounded as $z \rightarrow -\infty$ is

$$p_0(z) = C s(z), \quad (1.56)$$

where

$$s(z) \equiv \exp(-\frac{1}{3}z^3 - 2Ez) \int_{-\infty}^z \exp(\frac{1}{3}u^3 + 2Eu) du. \quad (1.57)$$

The constant C is determined by the normalization condition, Eq. (1.48). This gives

$$C = \left[\int_{-\infty}^{\infty} s(z) dz \right]^{-1}. \quad (1.58)$$

When $(z^2 + 2E)$ is large compared to 1, $s(z)$ may be expanded as

$$s(z) \sim (z^2 + 2E)^{-1} + 2z(z^2 + 2E)^{-3} + \dots \quad (1.59)$$

It follows that

$$\lim_{z \rightarrow \pm\infty} z^2 s(z) = 1, \quad (1.60)$$

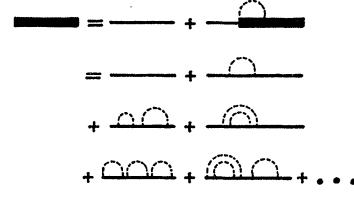


FIG. 3. Self-consistent Green's function approximation. Heavy solid line denotes complete Green's function for particle; light solid line denotes unperturbed Green's function for particle; dotted line denotes a phonon (Ref. 11) or connects repeated scattering from same impurity (Ref. 12).

and from (1.52) we see that the constant C is just the cumulative density of states, $N(E)$. Hence, substituting (1.57) in (1.58), we find, after changing variables and performing one integration,

$$N(E) = \left[\int_0^{\infty} \pi^{1/2} u^{-1/2} \exp(-\frac{1}{12}u^3 - 2Eu) du \right]^{-1}, \quad (1.61)$$

which is a result obtained by Frisch and Lloyd. In Appendix B we show, by working with the Fourier transform of p_0 , that the cumulative density of states can also be expressed as

$$N(E) = \pi^{-2} \{ [\text{Ai}(-2E)]^2 + [\text{Bi}(-2E)]^2 \}^{-1}, \quad (1.62)$$

where Ai and Bi are the well-known Airy functions.¹³

From either (1.61) or (1.62), we may establish the asymptotic forms:

$$N(E) \sim (2E)^{1/2} \pi^{-1}, \quad \text{for } E \gg 0, \quad (1.63)$$

$$N(E) \sim |2E|^{1/2} \pi^{-1} \exp(-\frac{4}{3}|2E|^{3/2}), \quad \text{for } E \ll 0. \quad (1.64)$$

Equation (1.63) is just the result one would obtain in the absence of the random potential, and is the result one expects from perturbation theory. Equation (1.64), however, cannot be obtained by such simple methods.

In order to find $A(k, E)$, it is necessary to know $p_1(z)$ as well as p_0 . Unfortunately, no explicit solution of Eq. (1.47) has been found. It has been possible, however, to find simple analytic expressions for the asymptotic forms of the spectral density, when one of the variables k and E remains fixed and the other approaches infinity. Let us first consider the asymptotic forms of $A(0, E)$ when E approaches $\pm\infty$. When $E \gg 0$, p_0 can be expanded in the form of Eq. (1.59). We may obtain a similar asymptotic expansion for $p_1(z)$ by treating the diffusion term in (1.47) as a small perturbation, and expanding p_1 in powers of this perturbation, using, at the same time, the expansion for p_0 . We find

$$p_1(z) \sim -N(E) \left[\frac{z}{2E(z^2 + 2E)} + \frac{z^2 - 4E}{3E(z^2 + 2E)^3} + \dots \right]. \quad (1.65)$$

¹³ J. C. P. Miller, *The Airy Integral*, British Association for the Advancement of Science Mathematics Tables (University Press, Cambridge, England, 1946), Part B.

Substitution of the expansions for p_0 and p_1 in (1.49) gives the asymptotic form for the spectral density:

$$A(0,E) \sim 2^{-3/2} \pi^{-1} E^{-5/2}, \quad \text{for } E \gg 0. \quad (1.66)$$

This is in agreement with the results of perturbation theory.

The form of $A(0,E)$, when $E \ll 0$, is considerably harder to obtain. One may proceed by first finding two independent solutions, in the limit $E \ll 0$, of the homogeneous equation

$$[(d^2/dz^2) + (z^2 + 2E)(d/dz) + z]f(z) = 0. \quad (1.67)$$

From the two solutions of the differential equation, one can construct the Green's function for the differential operator on the right-hand side, with the boundary condition

$$\lim_{z \rightarrow +\infty} zf(z) = \lim_{z \rightarrow -\infty} zf(z). \quad (1.68)$$

Applying the Green's function to the known function $p_0(z)$, one obtains the function $p_1(z)$, and thence, the asymptotic form of $A(0,E)$.

The form of the solutions of (1.67) can best be understood by writing

$$f(z) \equiv \exp(-\frac{1}{6}z^3 - Ez)u(z). \quad (1.69)$$

Equation (1.66) then assumes the more familiar form

$$[-(d^2/dz^2) + \frac{1}{4}(z^2 + 2E)^2]u(z) = 0, \quad (1.70)$$

which is the Schrödinger equation for a particle in a certain quartic potential. For $E \ll 0$, $u(z)$ may be approximated by the WKB method. The points $z = \pm |2E|^{1/2}$ are second-order classical turning points, and the appropriate connecting functions must be used in the vicinity of these points.¹⁴ The result of these calculations is that the spectral density has the asymptotic form

$$A(0,E) \sim 2\pi |2E|^{1/2} \exp(-\frac{4}{3}|2E|^{3/2}), \quad \text{for } E \ll 0. \quad (1.71)$$

Although the asymptotic forms for $A(k,E)$ given by (1.66) and (1.71) were derived for $k=0$, it is not difficult to verify that the same results hold for $k \neq 0$, provided that k is held constant while $|E|$ becomes sufficiently large. The asymptotic form, when $E \rightarrow -\infty$ and $k/|E|^{1/2}$ approaches a finite, nonzero constant, is also of interest. It may be obtained by a procedure very similar to that leading to Eq. (1.71), for the case of $k=0$. The result is that $A(k,E) \sim A(0,E) \times \text{sech}^2(\pi k/|8E|^{1/2})$.

The asymptotic form, when $k \rightarrow \infty$ while E is held fixed, can be found by expanding the solution of Eq. (1.47) for $p_1(z)$ in powers of k^{-1} . The fourth term in the expansion is the first which contributes to the integral (1.49) for $A(k,E)$. and, using the relation (1.55), it can be shown that for sufficiently large k ,

$$A(k,E) \sim 2k^{-4} \rho(E). \quad (1.72)$$

This asymptotic form of the spectral density, for large k , may also be obtained by perturbation-theoretic arguments.

Other Potentials

The essential property of the equations of motion for z and U_1 which permitted us to write down an equation of motion for the joint probability distribution $P(z, U_1; x)$ was that the quantities $z(x; E)$ and $U_1(x; E)$ form a Markoff process, as x moves from left to right along the line. If, instead of the Gaussian-white-noise potential, we had used a model, such as Frisch and Lloyd's, of δ -function potentials scattered independently at random on the line, the Markoff property would still hold and the procedures of this section could be carried out. If the "impurity" potentials had nonzero range, however, $z(x; E)$ and $U_1(x; E)$ would not form a continuous Markoff process. If one considers any model in which various kinds of "impurity" potentials of finite spatial extent occur in random sequence on a line, with a given distribution of possible distances between successive impurity potentials, and zero probability of overlap between two potentials, one can obtain a discrete Markoff process by considering the values of z and U_1 at the right-hand side of each impurity potential. One can obtain a similar discrete Markoff process for a sequence of finite potential wells of random depth.

The condition which enabled us to work with the functions $P_s(z; x)$, instead of the joint distribution of z and U_1 , was that the equation of motion for U_1 was linear in U_1 . This condition also applies to the more general models of the preceding paragraph. It follows that the spectral density of such a system is accessible to the general methods of this paper. The mathematical details of such a calculation are very similar to the procedures to be discussed in Secs. 2 and 3 of this paper, and we shall not examine them further.

2. DISCRETE PARTICLES

The Model

As another application of the general method, we calculate the spectral density for a model of a particle in an energy band in a discrete lattice. We may imagine the particle to be a conduction electron or a tightly bound exciton in a chain of N identical atoms of infinite mass, the random part of the particle Hamiltonian arising from thermal fluctuations in the distances between neighboring atoms. The electronic state of the system is described by giving the probability amplitude $\psi(m)$ for finding the particle at each lattice site, $1 \leq m \leq N$. We assume that the particle Hamiltonian H is of the form

$$H\psi(m) \equiv K_m\psi(m) + M_{m-1}\psi(m) + M_m\psi(m+1), \quad \text{for } 2 \leq m \leq N-1. \quad (2.1)$$

The diagonal matrix element K_m is assumed to depend linearly on h_m and h_{m-1} , the deviations from equilibrium

¹⁴ L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), pp. 184-192.

of the distances between atom m and its nearest neighbors, atom $m+1$ and atom $m-1$, respectively. The off-diagonal element M_m is assumed to be a linear function of the distance between atoms m and $m+1$. Thus we may write

$$K_m \equiv E_0 + \alpha h_m + \alpha h_{m-1}, \quad (2.2)$$

$$M_m \equiv M + \beta h_m. \quad (2.3)$$

We assume all quantities in (2.2) and (2.3) to be real.

If the atoms of the lattice are connected with springs between nearest neighbors only, we know from classical statistical mechanics that the distributions of the various h_m are statistically independent. If the springs are perfectly harmonic, then the distribution of each h_m is a Gaussian distribution with mean zero and variance $k_B T a / B$, where T is the temperature, a is the equilibrium interatomic distance, and B is the elastic modulus of the chain.

The spectral density is defined as

$$A(q, E) \equiv N^{-1} \left\langle \sum_i \left| \sum_{m=1}^N e^{-iqm} \psi_i(m) \right|^2 \delta(E - E_i) \right\rangle, \quad (2.4)$$

where E_i and ψ_i are the i th eigenvalue and eigenfunction of the Hamiltonian, the eigenfunction being normalized by

$$\sum_{m=1}^N |\psi_i(m)|^2 = 1. \quad (2.5)$$

To completely specify the Hamiltonian (2.1), we must specify the values of $H\psi(m)$ at the endpoints $m=1$ and $m=N$. For a perfect lattice ($h_m \equiv 0$), it is convenient to assume periodic boundary conditions. In that case, the eigenstates of the Hamiltonian are periodic waves,

$$\psi_q(m) = N^{-1/2} e^{iqm}, \quad (2.6)$$

for $q=0, \pm 2\pi N^{-1}, \pm 4\pi N^{-1}$, etc., with energies

$$E_q = E_0 + 2M \cos q. \quad (2.7)$$

For our present purposes, we shall not use periodic boundary conditions, but shall specify the boundary conditions by defining quantities $\psi(0)$, $\psi(N+1)$, h_0 and h_N to be substituted in Eq. (2.1) at the end points. We define

$$\psi(0) \equiv y_0 M^{-1} \psi(1), \quad (2.8)$$

$$h_0 \equiv 0, \quad (2.9)$$

$$\psi(N+1) \equiv (M + \beta h_N) (y_N - \alpha h_N)^{-1} \psi(N), \quad (2.10)$$

where y_0 and y_N are real fixed constants. We shall not fix the quantity h_N , however, but shall consider a statistical ensemble of crystals, in which h_N is a random variable which is statistically independent of the other h_m and has the same probability distribution as each of the h_m . When the number of atoms is large, of course, the spectral density will be independent of the choice of boundary condition.

The relation between the discrete Hamiltonian of the present section and the Schrödinger Hamiltonian of Sec. 1 may be seen, if one assumes that the wave functions of interest are slowly varying functions of m . The finite difference operator H can then be approximated by a differential operator, which, for the case of a perfect lattice, is the Schrödinger Hamiltonian for a free particle with effective mass $m^* = -2\hbar^2 / M a^2$. For the imperfect lattice, we have the additional terms αh_m and βh_m of Eqs. (2.2) and (2.3). The first of these leads to a deformation potential, while the second leads to a combination deformation potential and local change of effective mass. If the wave functions are sufficiently slowly varying, and the perturbation sufficiently weak, the local change of effective mass will be negligible compared to the deformation potential. The value of the deformation potential coefficient V_0 , as defined by Eq. (1.6), is given for the present model by

$$V_0 = (2\alpha + 2\beta)a. \quad (2.11)$$

In the limit of slowly varying wave functions, the effect of the deformation potential is the same as that of a Gaussian white-noise potential, with coefficient D given, as for the continuous string, by

$$D = 2V_0 k_B T / B. \quad (2.12)$$

Although the equations for $A(q, E)$ given below are derived for general values of the parameters, numerical computations have been carried out only for the case of β and q equal to zero. To facilitate comparison with the results of Sec. 1, the units of length, time, and mass were again chosen such that $\hbar = m^* = D = 1$, with D defined by (2.12) and (2.11). Also to facilitate comparisons, the origin of the energy scale was chosen to be the edge of the unperturbed energy band, so that $E_0 + 2M = 0$. The dimensionless parameter which controls the shape of the spectral density is the lattice constant a , expressed in terms of the unit of length, $\kappa_0^{-1} = (D m^* \hbar^{-4})^{-1/3}$.

The function $A(0, E)$ is plotted, for several values of the lattice parameter a , in Fig. 4. The value $a=0$ corresponds to the continuous model of Sec. 1. The limit $a \gg \kappa_0^{-1}$ corresponds to an energy bandwidth ($|4M| = 2\hbar^2 |m^*|^{-1} a^{-2}$) which is small compared with the root-mean-square deformation potential. In such a system, the eigenstates are localized at a single lattice site m , and the energy is shifted by the deformation potential at that site, $\alpha(h_m + h_{m-1})$. This leads to a spectral density, independent of the wave number q , which is a Gaussian distribution with variance equal to $D/4a$.^{15,16} When a is not large compared to κ_0^{-1} ,

¹⁵ The Gaussian shape for the spectral density in the limit of zero bandwidth is derived in Ref. 8 by summation of the perturbation theory expansion for the Green's function.

¹⁶ When the bandwidth is zero, it is possible to calculate the spectral density exactly, even when phonon energies are not zero. See, J. J. Hopfield, in International Conference on the Physics of Semiconductors, Exeter, 1962 (The Institute of Physics and the Physical Society, London, 1962), p. 75; M. Lax, J. Chem. Phys. 20, 1752 (1952).

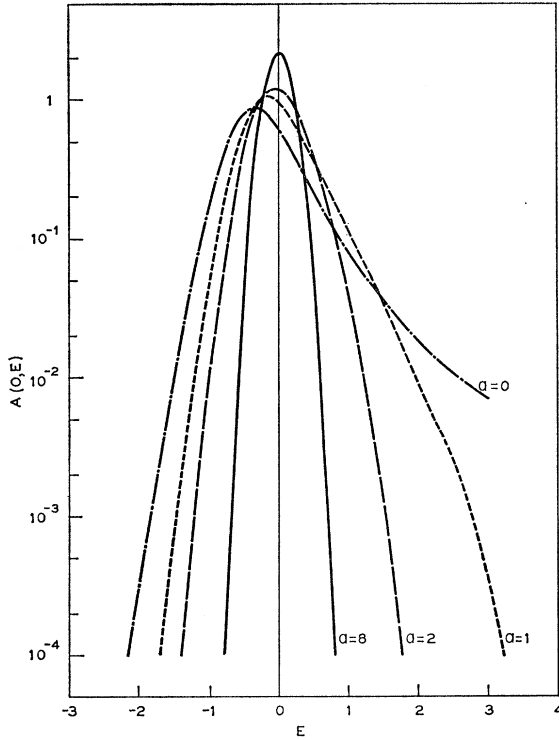


FIG. 4. The spectral density $A(0,E)$ for the discrete model, for several values of the lattice constant a . The energy E is measured in units of $\epsilon_0 = (D^2 m^* \hbar^{-2})^{1/3}$; the lattice constant in units of $\kappa_0^{-1} = (D m^* \hbar^{-4})^{-1/3}$. The zero of energy is the energy of the $k=0$ state in the unperturbed lattice.

the spectral density still has the Gaussian form, $\text{const} \times \exp[-2(E-E_0)^2 a/D]$, whenever the magnitude of $(E-E_0)$ is large compared to the bandwidth. Note that the center of this Gaussian is the *center* of the unperturbed band. In Fig. 4, the curve corresponding to $a=8$ is almost undistinguishable from a Gaussian.

Procedure

For each energy, and each lattice configuration, we define a function $\varphi(m)$, such that $\varphi(0)=1$, $\varphi(m)$ obeys the homogeneous "initial condition" (2.8), and φ obeys the difference equation

$$M_m \varphi(m+1) + M_{m-1} \varphi(m-1) + (K_m - E) \varphi(m) = 0. \quad (2.13)$$

We define

$$y(m) \equiv (M + \beta h_{m-1}) \varphi(m-1) / \varphi(m) + \alpha h_{m-1}. \quad (2.14)$$

The "initial condition" (2.8) implies that

$$y(1) = y_0. \quad (2.15)$$

The final condition (2.10) means that E is an eigenvalue of the Hamiltonian, if and only if

$$y(N+1) = y_N. \quad (2.16)$$

We also define

$$U_1(m) \equiv \sum_{m'=1}^{m-1} \frac{e^{-iqm'} \varphi(m')}{e^{-iqm} \varphi(m)}, \quad (2.17)$$

$$U_2(m) \equiv \sum_{m'=1}^{m-1} \frac{\varphi(m')^2}{\varphi(m)^2}, \quad (2.18)$$

$$U_3(m) \equiv (\partial/\partial E)y(m). \quad (2.19)$$

The functions y and U obey the equations

$$y(m+1) = \alpha h_m - (M + \beta h_m)^2 \times [y(m) + \alpha h_m - E + E_0]^{-1}, \quad (2.20)$$

$$U_1(m+1) = e^{iq} [U_1(m) + 1] \times [y(m+1) - \alpha h_m] (M + \beta h_m)^{-1}, \quad (2.21)$$

$$U_2(m+1) = [U_2(m) + 1] \times [y(m+1) - \alpha h_m]^2 (M + \beta h_m)^{-2}, \quad (2.22)$$

$$U_3(m+1) = [U_3(m) - 1] \times [y(m+1) - \alpha h_m]^2 (M + \beta h_m)^{-2}. \quad (2.23)$$

The three functions $U(m)$ are equal to zero when $m=1$. Hence, comparing (2.22) and (2.23) we see that for all m ,

$$U_2(m) = -U_3(m). \quad (2.24)$$

The spectral density is then given by

$$A(q,E) = N^{-1} \langle |U_1(N+1)|^2 / U_2(N+1) \times |U_3(N+1)| \delta[y_N - y(N+1)] \rangle = N^{-1} \langle |U_1(N+1)|^2 \delta[y_N - y(N+1)] \rangle. \quad (2.25)$$

We define the functions $P_s(y; m)$ as

$$P_s(y; m) = \langle U_1(m)^s \delta[y - y(m)] \rangle, \quad \text{for } s=0, 1 \\ = \langle |U_1(m)|^2 \delta[y - y(m)] \rangle, \quad \text{for } s=2. \quad (2.26)$$

These obey equations of motion of the form

$$P_0(y; m+1) = \int_{-\infty}^{\infty} F_0(y, y') P_0(y'; m) dy', \quad (2.27)$$

$$P_1(y; m+1) = e^{iq} \int_{-\infty}^{\infty} F_1(y, y') \times [P_1(y'; m) + P_0(y'; m)] dy', \quad (2.28)$$

$$P_2(y; m+1) = \int_{-\infty}^{\infty} F_2(y, y') [P_2(y'; m) + 2 \text{Re} P_1(y'; m) + P_0(y'; m)] dy'. \quad (2.29)$$

The kernels $F_s(y, y')$ are given, in terms of the probability distribution $p(h)$ obeyed by each of the h_m , by the

equation

$$F_s(y, y') = \int \left(\frac{y - \alpha h}{M + \beta h} \right)^s \times \delta \left[y - \alpha h - \frac{(M + \beta h)^2}{y' - \alpha h - E + E_0} \right] p(h) dh. \quad (2.30)$$

The behavior of $P_s(y; m)$ for large m may be studied by a procedure very similar to the analysis of the corresponding quantities for the white-Gaussian-noise potential given in Appendix A. We use the fact that the integral operator on the right-hand side of (2.29) is related by a change of variables to the adjoint of the operator in (2.27), a fact which follows from the relation

$$F_2(y, y') = F_0(E - E_0 - y', E - E_0 - y). \quad (2.31)$$

The functions $P_0(y; m)$ and $P_1(y; m)$ approach functions $p_0(y)$ and $p_1(y)$, independent of m , when m becomes large. These limiting functions may be determined by substituting p_0 and p_1 for P_0 and P_1 on both sides of (2.27) and (2.28), and using the fact that p_0 , as a probability distribution, is normalized to have area one. When m is large, the function $P_2(y; m)$ has the asymptotic form, $\text{const} \times m + f(y)$. The resulting spectral density, for large N , is independent of N and y_N , and is given by

$$A(q, E) = \int_{-\infty}^{\infty} p_0(E - E_0 - y) \times [2 \text{Re} p_1(y) + p_0(y)] dy. \quad (2.32)$$

Thus, the problem of finding the spectral density is reduced to the solution of two one-dimensional integral equations, for p_0 and p_1 , and one quadrature.

3. PHONON GREEN'S FUNCTIONS

The similarity between problems involving normal modes of phonons and those involving electronic eigenstates has been emphasized by Schmidt.² It is not surprising, therefore, that the methods of the previous sections may be used to find phonon Green's functions for certain one-dimensional models. We shall consider here a model in which N atoms on a line are connected to their nearest neighbors by identical harmonic springs with spring constant K . The mass of each atom may be any one of the values M_1, M_2, \dots ; the probability that mass of the m th atom, μ_m , has the value M_r is w_r , and is independent of all the other masses on the line. The functions we are interested in are correlation functions of the form

$$D(q, \omega) = \int_{-\infty}^{\infty} e^{i\omega t} \langle \langle X_q(t) X_q^\dagger(0) \rangle \rangle dt, \quad (3.1)$$

where we have used the double angular bracket $\langle \langle \dots \rangle \rangle$ to indicate the quantum-mechanical expectation value for a variable, averaged over the thermal distribution of phonon occupation numbers, as well as over the possible sequences of the different masses. The variables

X_q are defined as

$$X_q = N^{-1/2} \sum_{m=1}^N e^{-iqm} \lambda_m R_m, \quad (3.2)$$

where R_m is the displacement of the m th atom from equilibrium and λ_m is a real or complex number which depends on the particular type of atom at the m th site. For example, in applications to the one-phonon inelastic scattering of neutrons,¹⁷ λ_m would be the scattering length of the m th atom. To each value of the mass M_r there is a corresponding value Λ_r , so that $\lambda_m = \Lambda_r$ whenever $\mu_m = M_r$. The operator R_m may be expanded in terms of the normal coordinates Q_i of the crystal as

$$R_m = \sum_i u_i(m) Q_i, \quad (3.3)$$

where $u_i(m)$ is the eigenfunction for the i th normal mode. The function $D(q, \omega)$ may then be expressed as

$$D(q, \omega) = \pi \hbar |\omega|^{-1} n(\omega) A(q, |\omega|), \quad (3.4)$$

where

$$n(\omega) \equiv [\exp(\hbar\omega/k_B T) - 1]^{-1} + 1, \quad \text{for } \omega > 0, \\ \equiv [\exp(\hbar|\omega|/k_B T) - 1]^{-1}, \quad \text{for } \omega < 0, \quad (3.5)$$

and the spectral density $A(q, \omega)$ is defined by

$$A(q, \omega) \equiv N^{-1} \langle \sum_i | \sum_{m=1}^N e^{iqm} \lambda_m u_i(m) |^2 \delta(\omega - \omega_i) \rangle, \quad (3.6)$$

where ω_i is the frequency of the i th mode. The eigenfunctions $u_i(m)$ obey the equations

$$K u_i(m+1) + K u_i(m-1) - (2K - \mu_m \omega_i^2) u_i(m) = 0, \quad (3.7)$$

$$\sum_{m=1}^N \mu_m u_i(m)^2 = 1. \quad (3.8)$$

The u_i must obey appropriate homogeneous boundary conditions at the ends of the line, which we shall not specify here.

In order to simplify slightly the equations which follow, we assume that units have been chosen such that the spring constant K equals one.

In the analogy with the procedures of Secs. 1 and 2, we define for each frequency $\omega > 0$, and for each of the possible sequences of masses, a function $\varphi(m)$, which has a fixed value at $m=0$, which obeys the homogeneous boundary condition at the left-hand end of the chain, and which obeys the difference equation of (3.7) with ω and φ substituted for ω_i and u_i . Let us also define

$$y(m) = \varphi(m-1)/\varphi(m), \quad (3.9)$$

$$U_1(m) = \sum_{m'=1}^{m-1} \frac{\lambda_{m'} e^{-iqm'} \varphi(m')}{e^{-iqm} \varphi(m)}, \quad (3.10)$$

$$U_2(m) = \sum_{m'=1}^{m-1} \frac{\mu_{m'} \varphi(m')^2}{\varphi(m)^2}, \quad (3.11)$$

$$U_3(m) = (\partial/\partial\omega) y(m). \quad (3.12)$$

¹⁷ See C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), Chap. 19.

These obey the equations

$$y(m+1)=[2-\mu_m\omega^2-y(m)]^{-1}, \quad (3.13)$$

$$U_1(m+1)=e^{i\alpha}y(m+1)[U_1(m)+\lambda_m], \quad (3.14)$$

$$U_2(m+1)=y(m+1)^2[U_2(m)+\mu_m], \quad (3.15)$$

$$U_3(m+1)=y(m+1)^2[U_3(m)+2\mu_m\omega]. \quad (3.16)$$

From the last two equations we see that

$$U_3(m)=2\omega U_2(m). \quad (3.17)$$

If we define $P_s(y; m)$ precisely as in Eq. (2.26), then

$$A(q, \omega)=2\omega N^{-1}P_2(y_N; N), \quad (3.18)$$

where we have assumed a boundary condition on the right-hand end of the chain of form $y(N+1)=y_N$. The equations of motion for the P_s are

$$P_0(y; m+1)=y^{-2}\sum_r w_r P_0(2-M_r\omega^2-y^{-1}; m), \quad (3.19)$$

$$P_1(y; m+1)=e^{i\alpha}y^{-1}\sum_r w_r [P_1(2-M_r\omega^2-y^{-1}; m) + \Lambda_r P_0(2-M_r\omega^2-y^{-1}; m)], \quad (3.20)$$

$$P_2(y; m+1)=\sum_r w_r \{P_2(2-M_r\omega^2-y^{-1}; m) + 2 \operatorname{Re}[\Lambda_r P_1(2-M_r\omega^2-y^{-1}; m)] + |\Lambda_r|^2 P_0(2-M_r\omega^2-y^{-1}; m)\}. \quad (3.21)$$

If the functions $P_0(y; m)$ and $P_1(y; m)$ approach continuous limits $p_0(y)$ and $p_1(y)$, as $m \rightarrow \infty$, then these limits can be found by substituting p_s for P_s on both sides of Eqs. (3.19) and (3.20). If, furthermore, the function $P_2(y; m)$ has the asymptotic form, $\text{const} \times m + f(y)$, as $m \rightarrow \infty$, then we may find the spectral density by multiplying both sides of Eq. (3.21) by $\sum_r w_r p_0(2-M_r\omega^2-y)$ and integrating with respect to y . By changing the variable of integration on the right-hand side from y to $Y=2-M_r-y^{-1}$, and using the difference equation satisfied by p_0 , we find (in the limit $N \rightarrow \infty$)

$$A(q, \omega)=2\omega \int_{-\infty}^{\infty} \sum_r w_r p_0(2-M_r-Y) \times \{2 \operatorname{Re}[\Lambda_r p_1(Y)] + |\Lambda_r|^2 p_0(Y)\} dY. \quad (3.22)$$

Unfortunately, the functions $P_s(y; m)$ do not necessarily approach continuous limits as $m \rightarrow \infty$, even if one starts with a continuous function for $P_0(y; 0)$. Schmidt² showed that, at least in certain cases, $p_0(y)$, if it exists at all, is highly discontinuous, the values of $p_0(y)$ being infinite at a dense set of points. Even if the limit $p_0(y)$ does exist, in these cases, it is not clear that the limit $p_1(y)$ will exist, or that the integral on the right-hand side of (3.22) will exist. In fact, there is reason for believing that $A(q, \omega)$ itself is infinite at a dense set of points in certain regions of the line $0 < \omega < \infty$, while the integral $\int_0^\omega A(q, \omega') d\omega'$ is a continuous function of ω . Numerical computations of

$A(q, \omega)$ in these regions of bad behavior is clearly out of the question.

The reason for this difficulty is that we have chosen a discrete set of masses M_r . If we had chosen a continuous distribution of possible masses, so that the sums in Eqs. (3.19)–(3.22) were changed to integrals, then all the limits would have existed and the functions p_s would be continuous. Physically, we expect to be able to approximate a discrete distribution as closely as we desire by a continuous distribution which is sharply peaked about the values of the discrete distribution. If $A(q, \omega)$ is discontinuous for the discrete distribution, we would not expect to be able to calculate it in this manner; but the quantities of real physical interest are averages of the spectral density over a finite spread of ω , such as $(\Delta\omega)^{-1} \int_{\omega-\Delta\omega}^{\omega+\Delta\omega} A(q, \omega') d\omega'$, and we do expect that, for fixed $\Delta\omega$, such quantities can be calculated as accurately as desired by choosing a continuous distribution sufficiently close to the discrete distribution.

4. TWO-PARTICLE FUNCTIONS

Electrical Conductivity

The methods of the previous sections can be generalized to two-particle functions, such as the frequency-dependent electrical conductivity of a system of noninteracting electrons in a random potential. The real part of the conductivity, at frequency ω , for a collection of noninteracting, spinless particles of charge e and mass m , is given by¹⁸

$$\operatorname{Re}\sigma(\omega)=\frac{\pi e^2}{m^2} \int_{-\infty}^{\infty} \frac{f(\hbar\nu)-f[\hbar(\nu+\omega)]}{\hbar\omega} F(\nu, \nu+\omega) d\nu, \quad (4.1)$$

where f is the Fermi function,

$$f(E)\equiv\{\exp[(E-\mu)/k_B T]+1\}^{-1}, \quad (4.2)$$

and F is defined by

$$F(\nu, \nu')\equiv L^{-1} \left\langle \sum_{ij} |(i|p|j)|^2 \delta\left(\nu-\frac{E_i}{\hbar}\right) \delta\left(\nu'-\frac{E_j}{\hbar}\right) \right\rangle. \quad (4.3)$$

In Eq. (4.3), L is the length of the system, $(i|p|j)$ is the matrix element of the momentum operator between the eigenstates i and j of the one-particle Hamiltonian, and E_i and E_j are the energies of the eigenstates; the quantity μ in Eq. (4.2) is the chemical potential of the electron system. If the real part of the conductivity is known, the imaginary part may be calculated by use of the Kramers-Kronig relations.

As an example, we shall derive the expressions for F when the random potential is the white-Gaussian-noise potential of Sec. 1. We again choose units such that $\hbar=m=D=1$. We define the functions $\varphi(x; E)$ and

¹⁸ See H. Nakano, Progr. Theoret. Phys. (Kyoto) **15**, 77 (1956).

$z(x; E)$ as in Sec. 1. We also define a new function

$$W(x; E, E') \equiv \frac{\int_0^x \varphi(x'; E) \frac{\partial}{\partial x'} \varphi(x'; E') dx'}{\varphi(x; E) \varphi(x; E')}. \quad (4.4)$$

The equation of motion for W is

$$\partial W / \partial x = z(x; E') - [z(x; E') + z(x; E)] W. \quad (4.5)$$

Functions $P_s(z, z'; x)$ are defined, for $s=0, 1, 2$, by

$$P_s(z, z'; x) \equiv \langle W(x; E, E')^s \delta[z - z(x; E)] \times \delta[z' - z(x; E')] \rangle. \quad (4.6)$$

The equations of motion for these functions are

$$\frac{\partial P_s}{\partial x} = \left[\frac{\partial^2}{\partial z^2} + 2 \frac{\partial^2}{\partial z \partial z'} + \frac{\partial}{\partial z^2} + (z^2 + 2E) \frac{\partial}{\partial z} + (z'^2 + 2E') \frac{\partial}{\partial z'} + (2-s)(z+z') \right] P_s + s z P_{s-1}. \quad (4.7)$$

[Note that the "diffusion term,"

$$\frac{\partial^2}{\partial z^2} + 2 \frac{\partial^2}{\partial z \partial z'} + \frac{\partial^2}{\partial z'^2},$$

represents random walk in the $(z+z')$ direction only; the random potential in the equation of motion for $z(x; E)$ is the same as that in the equation for $z(x; E')$.] The boundary conditions at infinity on the functions P_s are

$$\begin{aligned} \lim_{z \rightarrow +\infty} z^{2-s} P_s &= \lim_{z \rightarrow -\infty} z^{2-s} P_s, \\ \lim_{z' \rightarrow +\infty} z'^{2-s} P_s &= \lim_{z' \rightarrow -\infty} z'^{2-s} P_s. \end{aligned} \quad (4.8)$$

If E does not equal E' , then P_0 and P_1 approach limits $p_0(z, z')$ and $p_1(z, z')$, independent of x , as x approaches infinity. The limiting functions are determined by the differential equations (4.7), with the left-hand sides set equal to zero, together with the boundary conditions (4.8) and the normalization condition $\int \int p_0(z, z') dz dz' = 1$. The function P_2 has the asymptotic form, $\text{const} \times x + f(z, z')$, and we find that in the limit of very large L ,

$$\begin{aligned} F(E, E') &= 4L^{-1} P_2(z_L, z_L; L) \\ &= 8 \int \int p_0(-z, -z') p_1(z, z') z dz dz'. \end{aligned} \quad (4.9)$$

For the case where $E=E'$, these methods cannot be used directly, because p_0 and p_1 do not then approach a well-behaved limit as $x \rightarrow \infty$. The zero-frequency conductivity must therefore be obtained by studying the limit of $\sigma(\omega)$ as $\omega \rightarrow 0$.

Interband Optical Transitions

As a final example of the properties which can be calculated using the methods of this paper, we mention the line shape for optical absorption by interband electronic transitions, under the assumption that the electron and hole do not interact. We consider a model in which the electron and hole are treated in the effective mass approximation, and the random potential is white Gaussian noise arising from a deformation potential on a classical continuous string. The effective mass m^* and the deformation potential coefficient V_0 may be different for the electron and hole. We assume that the interband part of the momentum operator, which is responsible for the interband transitions, has the form

$$\begin{aligned} \hat{p}_{\text{interband}} &= \text{const} \\ &\times \int [a_h^\dagger(x) a_e^\dagger(x) + a_e(x) a_h(x)] dx, \end{aligned} \quad (4.10)$$

where a_h^\dagger , a_h , a_e^\dagger , and a_e are the creation and annihilation operators for a hole and an electron, respectively. The optical absorption for this model is proportional to

$$\alpha(\omega) \equiv \int G(\nu, \omega - \nu) d\nu, \quad (4.11)$$

where G is defined, in terms of φ_i^h and E_i^h , the wave function and energy of the i th hole eigenstate, and φ_j^e and E_j^e , the wave function and energy of the j th electron state, by

$$\begin{aligned} G(\nu, \nu') &\equiv L^{-1} \left\langle \sum_{ij} \left[\int_0^L \varphi_i^h(x) \varphi_j^e(x) dx \right]^2 \right. \\ &\quad \left. \times \delta\left(\nu - \frac{E_i^h}{\hbar}\right) \delta\left(\nu' - \frac{E_j^e}{\hbar}\right) \right\rangle. \end{aligned} \quad (4.12)$$

The procedures for calculating $G(\nu, \nu')$ are very similar to the methods used in calculating the function $F(\nu, \nu')$ of Eq. (4.3), and we shall not discuss them further here.

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APPENDIX A. ASYMPTOTIC BEHAVIOR OF $P_s(z; x)$

We wish to study the behavior, for large x , of the functions $P_s(z; x)$ for the Gaussian-white-noise potential of Sec. 1. The function P_0 is the probability distribution of $z(x; E)$, and we shall give a physical argument that this probability must approach a limiting distribution as $x \rightarrow \infty$. It is perhaps easiest to first project the

line $-\infty \leq z(x; E) \leq \infty$ onto the unit circle $0 \leq \theta(x) < 2\pi$ by

$$\theta(x) = 2 \arctan z(x; E). \tag{A1}$$

The equation of motion (1.20) for z can be translated into an equation of motion for $\theta(x)$, which may be described, like the equation for z , as a "flow" plus a "random walk." The flow velocity for θ is continuous at all points on the unit circle, including the point $\theta = \pi$, corresponding to $z = \infty$. The magnitude of the random walk vanishes at the point $\theta = \pi$, but the flow velocity at this point is not zero. At all other points on the circle, the random walk is nonzero. It is physically clear that no matter what the value is of $\theta(x)$, there will be a finite and nonvanishing probability density for $\theta(x + \Delta x)$ to be at any point on the circle, for any $\Delta x > 0$. More explicitly, we claim that for any $\Delta x > 0$, the conditional probability density $p(\theta' | \theta'', \Delta x)$, for $\theta(x + \Delta x)$ to have value θ' when $\theta(x) = \theta''$, is bounded above for all θ' and θ'' , and that there exists a lower bound $m > 0$ such that

$$p(\theta' | \theta'', \Delta x) \geq m, \quad \text{for all } \theta', \theta''. \tag{A2}$$

These conditions are more than sufficient to insure that the probability density of $\theta(x)$, and hence that of $z(x; E)$, approaches a limit exponentially fast as $x \rightarrow \infty$. It would have been sufficient for convergence that the above conditions hold for one particular $\Delta x > 0$. Also it would have been sufficient that (A2) hold for all θ'' , whenever θ' lies in a specified nonzero segment of the circle.¹⁹

The function $P_1(z; x)$ obeys the differential equation (1.40) with the boundary condition (1.35). Since the inhomogeneous term in (1.40), $P_0(z; x)$, approaches a limit exponentially fast, the function P_1 will approach a limit, if all solutions of the homogeneous equation

$$\frac{\partial}{\partial x} f(z; x) = \left[\frac{\partial^2}{\partial z^2} + (z^2 + 2E) \frac{\partial}{\partial z} + z - ik \right] f(z; x), \tag{A3}$$

with the boundary condition

$$\lim_{z \rightarrow +\infty} z f = \lim_{z \rightarrow -\infty} z f, \tag{A4}$$

decay to zero as $x \rightarrow \infty$. Let us define the function $U_4(x; E)$ by

$$U_4(x; E) \equiv c / e^{ikx} \varphi(x; E), \tag{A5}$$

where c is some constant. By examining the equation of motion for U_4 , one can readily see that the functions $f(z; x)$ are just the expectation values $\langle U_4(x; E) \times \delta[z - z(x; E)] \rangle$, where the average is to be taken not only over all potential configurations, but over a distribution of initial conditions z_0 and constants c , chosen so as to give the correct values for $f(z, 0)$. Using the

¹⁹ Cf. the discussion in Ref. 1, Appendix 2.

same reasoning as that used in Eq. (1.26), we see that

$$\begin{aligned} \langle U_4(L; E) \delta[z_L - z(L; E)] \rangle \\ = \frac{1}{2} e^{-ikL} \langle c \sum_i \psi_i(0) \psi_i(L) \delta(E - E_i) \rangle, \end{aligned} \tag{A6}$$

where the ψ_i are the normalized eigenstates of the Hamiltonian, with the boundary condition z_L . Borland²⁰ has shown that the eigenstates in a one-dimensional disordered potential are highly localized in space, decaying exponentially on either side of the point at which they are maximum. It follows that the product $\psi_i(0) \psi_i(L)$ will be very small for large L , and unless the density of states is infinite at energy E , the function $f(z_L; L)$ must be very small, for large L . Since z_L is an arbitrary constant, it follows that all solutions of (A3) and (A4) decay to zero as $x \rightarrow \infty$.

Finally, we consider $P_2(x; z)$. If the spectral density is to be independent of L , and of the boundary condition z_L , it follows that

$$x^{-1} P_2(z; x) = C + R(z, x), \tag{A7}$$

where C is a constant, and the remainder $R(z, x)$ vanishes as $x \rightarrow \infty$. If we make the further assumption that $x \partial R(z, x) / \partial x$ goes to zero for large x , then one can use the reasoning preceding (1.49) to evaluate C and thus determine the spectral density.

It is also possible to study the limiting form of P_2 more directly from the equation of motion (1.41), without use of the physical interpretation of P_2 . The function P_2 may be written as

$$P_2(z; x) = 2 \int_{-\infty}^{\infty} dz' \int_0^x dx' G(z, x - x'; z') \times \text{Re} P_1(z'; x'), \tag{A8}$$

where the Green's function $G(z, x; z')$ is the solution of the homogeneous equation

$$\frac{\partial}{\partial x} G(z, x; z') = \left[\frac{\partial^2}{\partial z^2} + (z^2 + 2E) \frac{\partial}{\partial z} \right] G(z, x; z'), \tag{A9}$$

for x greater than zero, with the boundary conditions

$$\lim_{z \rightarrow +\infty} G(z, x; z') = \lim_{z \rightarrow -\infty} G(z, x; z'), \tag{A10}$$

$$G(z, 0; z') = \delta(z - z'). \tag{A11}$$

We know that $P_1(z'; x')$ approaches a limit as $x \rightarrow \infty$; in order to find the asymptotic behavior of P_2 from (A8), we must also study the behavior of G . Let $H(z'; x; z)$ be the solution of the adjoint equations:

$$\frac{\partial H}{\partial x} = \left[\frac{\partial^2}{\partial z'^2} - \frac{\partial}{\partial z'} (z'^2 + 2E) \right] H, \quad \text{for } x > 0, \tag{A12}$$

$$\lim_{z' \rightarrow +\infty} z'^2 H = \lim_{z' \rightarrow -\infty} z'^2 H, \tag{A13}$$

$$H(z', 0; z) = \delta(z - z'). \tag{A14}$$

²⁰ R. E. Borland, Proc. Roy. Soc. (London) A274, 529 (1963).

If we multiply both sides of (A12) by $G(z', x'' - x; z'')$ and integrate with respect to z' and x , over the region $-\infty < z' < \infty$ and $0 \leq x \leq x''$, then we find, after integration by parts,²¹

$$G(z, x''; z'') = H(z'', x''; z). \tag{A15}$$

Note that Eq. (A12) is identical to the equation of motion (1.32) for P_0 except for the sign of z' . Hence, from our discussion of the limiting form of P_0 , it follows that $G(z, x; z')$ approaches the limit $p_0(-z')$ independent of the value of z as $x \rightarrow \infty$, and that this approach is exponentially fast. From this it follows that $P_2(z; x)$ has the form $(\text{const} \times x + f(z)) + \text{terms which go to zero as } x \rightarrow \infty$, and the spectral density, for large L , may be found from Eq. (1.49).

APPENDIX B. DENSITY OF STATES FOR THE WHITE-GAUSSIAN-NOISE POTENTIAL IN TERMS OF AIRY FUNCTIONS

Equation (1.46) for the probability distribution $p_0(z)$, in the case of a white-Gaussian-noise potential, may be integrated once with respect to z , giving

$$\left[\frac{d}{dz} + (z^2 + 2E) \right] p_0(z) = \text{const.} \tag{B1}$$

From Eq. (1.52) and the expansion in (1.59), we see that the constant in (B1) is just the cumulative density of states, $N(E)$. Taking the Fourier transform of (B1), we have

$$[-(d^2/dq^2) + iq + 2E] p(q) = 2\pi N(E) \delta(q), \tag{B2}$$

where $p(q)$ is the Fourier transform of $p_0(z)$. As a Fourier transform of a probability distribution, $p(q)$ must be equal to one when q equals zero, $p(q)$ must approach zero when $q \rightarrow \pm \infty$, and $p(q)$ must equal $p(-q)^*$.

²¹ Cf. B. Friedman, *Principles and Techniques of Applied Mathematics* (John Wiley & Sons, Inc., New York, 1956), p. 174.

This last requirement, together with (B2), implies that

$$-\lim_{q \rightarrow 0^+} \text{Re} d p(q) / dq = \pi N(E). \tag{B3}$$

If $g(q)$ is any solution of the homogeneous part of Eq. (B2), such that $g(q) \rightarrow 0$ as $q \rightarrow +\infty$, then it follows that $-\pi^{-1} \text{Re}[g'(0)/g(0)] = N(E)$. If we write $g(q) \equiv G(t)$, where $t = -iq - 2E$, we have

$$N(E) = -\pi^{-1} \text{Im}[G'(-2E)/G(-2E)]. \tag{B4}$$

The function $G(t)$ must approach zero as $t \rightarrow -i\infty$, and G must obey Airy's differential equation

$$G''(t) = tG(t). \tag{B5}$$

The general solution of (B5) is $G(t) = a \text{Ai}(t) + b \text{Bi}(t)$, where Ai and Bi are the Airy integrals, defined and tabulated for real values of t in Ref. 13. The Airy integrals may be expressed in terms of Bessel's functions of $\frac{1}{3}$ order, and have an analytic continuation to the entire complex plane. From the well-known asymptotic properties of the Bessel's functions,²² it follows that when $|t| \rightarrow \infty$, the Airy functions have the asymptotic form

$$\text{Ai}(-t) \sim \pi^{-1/2} t^{-1/4} \sin(\frac{1}{4}\pi + \frac{2}{3}t^{3/2}), \tag{B6}$$

$$\text{Bi}(-t) \sim \pi^{-1/2} t^{-1/4} \cos(\frac{1}{4}\pi + \frac{2}{3}t^{3/2}), \tag{B7}$$

in the sector $-\frac{2}{3}\pi < \arg t < \frac{2}{3}\pi$. The condition $G(t) \rightarrow 0$, as $t \rightarrow -i\infty$, thus implies

$$G(t) = a[\text{Ai}(t) - i \text{Bi}(t)]. \tag{B8}$$

Since the Wronskian, $\text{Ai}'(t) \text{Bi}(t) - \text{Bi}'(t) \text{Ai}(t)$, equals $-1/\pi$ for all t , we have, finally,

$$N(E) = \pi^{-2} \{ [\text{Ai}(-2E)]^2 + [\text{Bi}(-2E)]^2 \}^{-1}. \tag{B9}$$

²² E. Jahnke, F. Emde, and F. Lösch, *Tables of Higher Functions* (B. G. Teubner Verlagsgesellschaft, Stuttgart, 1960) 6th ed., p. 147.