Hopping conductivity of the Fibonacci-chain quasicrystal

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We present an exact calculation of the ac conductivity of a one-dimensional quasicrystal at all frequencies of the driving electric field. Our model is one of electrons tightly bound around identical atomic centers, with both the rates for hopping between adjacent sites and the distances between the sites varying quasiperiodically. The equations governing this system are the Miller-Abrahams equations, which we solve by a real-space renormalization-group method. We present results for the particular case of the "Fibonacci-chain" quasicrystal. Despite the strong similarity between the Miller-Abrahams equations and the equations previously used by other workers to find the electron and phonon spectra of similar systems, our results show none of the self-similar aspects displayed by those spectra. However, our results do corroborate earlier analytical results for the low- and high-frequency forms of the conductivity.

I. INTRODUCTION

In recent years considerable effort has been expended in the theoretical investigation of the properties of quasiperiodic systems, particularly since the discovery of real physical examples.[1] Much attention has been focused on the electron and phonon spectra of these systems, which display the self-similar form of a Cantor set.[2,3] More recently workers in the field have turned to the calculation of directly measurable quantities, such as the dynamic structure function[4] and the conductivity.[5] In 1988, Aldea and Dulea[6] showed that it is possible to derive the low- and high-frequency forms of the conductivity of a one-dimensional quasiperiodic lattice with electrons tightly bound around its atomic centers and gave results for three well-known quasi-lattices. In this article we give an exact solution of the equations governing this same problem using a real-space renormalization-group approach.

Though our method is, in theory, applicable to any of the quasiperiodic geometries explored by Aldea and Dulea, and indeed to any of the much larger class of geometries generated by discrete scaling or "inflation," we present the calculation only for the most famous example of a one-dimensional quasicrystal—the Fibonacci chain. This chain may be represented by the sequence of A's and B's generated as the limit of the repeated application of the (concurrent) "inflation rule,"

$$A \to AB \quad \text{and} \quad B \to A,$$

starting from a single letter A, where AB is the concatenation of A with B.

Our model is one in which atomic centers along a straight line are joined by links of two types, corresponding to the letters A and B in the Fibonacci chain. We study the infinite chain consisting of the periodic repetition of an arbitrarily high-order approximant to the Fibonacci chain. This approximant is formed by application of the inflation rules a finite number of times m to produce a chain of F_m links, where F_m is the mth Fibonacci number (with convention $F_1 = 2$). The Fibonacci chain itself is regarded as the limit of this chain as $m \to \infty$. Electrons are tightly bound around the sites in this lattice, and an electron may hop from one site to either of those adjacent as a result of interactions with a "bath" of lattice phonons in thermal equilibrium at a temperature T. Both the rates at which electrons hop along links and the lengths of the links are allowed to vary according to the pattern of A's and B's in the chain. A spatially constant electric field $E = E_0 e^{i\omega t}$ is applied along the line of the quasilattice, and the conductivity is determined by taking the spatial average of the current flowing between pairs of adjacent sites.

II. THE MILLER-ABRAHAMS EQUATIONS

The model we have described was studied by Miller and Abrahams in the late 1950s.[7] They derived equations whose solutions give the current flowing between any two sites in the lattice up to terms linear in the electric field. In the notation of the original article the equations linking the "voltage" variables V_n on the sites on a one-dimensional lattice are

$$i\omega C_n(V_n - Ex_n) = \frac{V_{n-1} - V_n}{Z_{n-1,n}} + \frac{V_{n+1} - V_n}{Z_{n,n+1}}. \quad (1)$$

Here x_n is the position of the nth site in the lattice and

$$C_n = \frac{e^2}{kT} f(E_n)[1 - f(E_n)],$$
$$\frac{1}{Z_{n,n+1}} = \frac{e^2}{kT} f(E_n)[1 - f(E_{n+1})]U_n,$$

where $f(\varepsilon)$ is the Fermi function, E_n is the energy of an electron localized about the nth site in the absence of an

electric field, and U_n is the width for a single electron to hop from the nth site to the $(n+1)$th in the absence of an electric field. If we can solve Eq. (1) for the voltage variables V_n given the rates U_n, then the conductivity of the model is given by

$$\sigma = \frac{1}{EL}\sum_n (x_{n+1}-x_n)\frac{V_{n+1}-V_n}{Z_{n,n+1}}, \tag{2}$$

where L is the length of the chain.

In our model, the E_n are all the same, so that $f(E_n)$ is a constant, independent of n, which simplifies the equations somewhat. Also, following Aldea and Dulea,[6] we can subtract each equation from the one immediately following it on the lattice and change to new variables

$$I_n = \frac{V_{n+1}-V_n}{Z_{n,n+1}}, \quad d_n = x_{n+1}-x_n,$$

which gives

$$\left(2+\frac{i\omega}{U_n}\right) I_n = I_{n-1} + I_{n+1} + i\omega E d_n. \tag{3}$$

The new variables have simple physical interpretations: I_n is the thermally averaged rate at which charge is transferred between the nth site and the $(n+1)$th, and d_n is the distance between nth site and the $(n+1)$th. In terms of the new variables the conductivity becomes

$$\sigma = \frac{1}{EL}\sum_n d_n I_n. \tag{4}$$

III. RENORMALIZATION-GROUP METHOD

On the Fibonacci chain the Miller-Abrahams equations take the form

$$\left(2+\frac{i\omega}{U_A}\right) I_n = I_{n-1} + I_{n+1} + i\omega E d_A, \tag{5}$$

on sites n followed by an A-type link, and

$$\left(2+\frac{i\omega}{U_B}\right) I_n = I_{n-1} + I_{n+1} + i\omega E d_B, \tag{6}$$

on sites n followed by a B-type one. These equations can be solved by a decimation process that is the exact reverse of the inflation process used to build up the chain.

The idea is that we divide our quasilattice into three sublattices called $\mathcal{L}_\alpha$, $\mathcal{L}_\beta$, and $\mathcal{L}_\gamma$ by labeling each site α, β, or γ, depending on what type of links it has to the left and to the right of it, as shown in Fig. 1. Then we treat the Miller-Abrahams equations as a special case of the more general set of equations

$$\epsilon_\alpha I_n = \gamma_A I_{n-1} + \gamma_A I_{n+1} + i\omega E h_\alpha, \quad n \in \mathcal{L}_\alpha, \tag{7}$$

$$\epsilon_\beta I_n = \gamma_A I_{n-1} + \gamma_B I_{n+1} + i\omega E h_\beta, \quad n \in \mathcal{L}_\beta, \tag{8}$$

$$\epsilon_\gamma I_n = \gamma_B I_{n-1} + \gamma_A I_{n+1} + i\omega E h_\gamma, \quad n \in \mathcal{L}_\gamma, \tag{9}$$

which develop under scaling. Clearly these are the same as the Miller-Abrahams equations provided we put

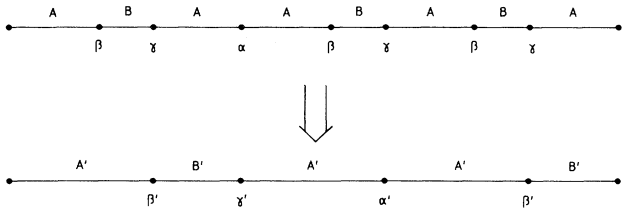

FIG. 1. Illustration of the decimation procedure for a chain of nine sites.

$$\begin{aligned} &\epsilon_\alpha = \epsilon_\gamma = 2 + \frac{i\omega}{U_A}, \quad \epsilon_\beta = 2 + \frac{i\omega}{U_B}, \\ &\gamma_A = \gamma_B = 1, \\ &h_\alpha = h_\gamma = d_A, \quad h_\beta = d_B. \end{aligned} \tag{10}$$

Reversing the inflation process (i.e., *deflating* the lattice),

$$AB \to A \text{ and } A \to B$$

is equivalent to removing all the β-type sites from the lattice (see Fig. 1), and eliminating from the equations all the variables I_n on those sites. When we do this we also relabel all the sites that remain α', β', or γ', according to the types (A or B) of their neighboring links in the renormalized lattice. These new site labels are not necessarily the same as the old ones.

The elimination of this subset of the variables I_n leaves us with a new set of equations linking the remaining variables that has exactly the same form as the old set, the only difference being that the eight parameters are renormalized thus:

$$\begin{aligned} &\epsilon'_\alpha = \epsilon_\gamma - \frac{\gamma_A^2+\gamma_B^2}{\epsilon_\beta}, \quad \epsilon'_\beta = \epsilon_\gamma - \frac{\gamma_B^2}{\epsilon_\beta}, \quad \epsilon'_\gamma = \epsilon_\alpha - \frac{\gamma_A^2}{\epsilon_\beta}, \\ &\gamma'_A = \frac{\gamma_A\gamma_B}{\epsilon_\beta}, \quad \gamma'_B = \gamma_A, \\ &h'_\alpha = h_\gamma + \frac{\gamma_A+\gamma_B}{\epsilon_\beta}h_\beta, \quad h'_\beta = h_\gamma + \frac{\gamma_B}{\epsilon_\beta}h_\beta, \\ &h'_\gamma = h_\alpha + \frac{\gamma_A}{\epsilon_\beta}h_\beta. \end{aligned} \tag{11}$$

The quantity we are currently interested in is the conductivity σ. Using Eqs. (11) and employing a few simple facts about the arrangement of α-, β-, and γ-type sites on the lattice, we can show that σ', the value of Eq. (4) on the decimated lattice, is given by

$$\sigma' = \sigma - i\omega\frac{N_\beta}{L}\frac{h_\beta^2}{\epsilon_\beta}, \tag{12}$$

where N_β is the number of β-type sites eliminated. Thus, by iterating this equation we find that

$$\sigma = \sigma^{(m)} + \frac{i\omega}{L}\sum_{l=0}^{m-1} N_\beta^{(l)}\frac{h_\beta^{(l)2}}{\epsilon_\beta^{(l)}}, \tag{13}$$

where $h_\beta^{(m)}, \epsilon_\beta^{(m)}, N_\beta^{(m)}$ denote the values of $h_\beta, \epsilon_\beta, N_\beta$ after m iterations of Eqs. (11).

So in order to calculate the conductivity of the chain for specific values of the quantities ω, U_A, U_B, d_A, and d_B, all we have to do is iterate Eq. (11) starting from the values (10) and accumulating the quantities $N_\beta h_\beta^2/\epsilon_\beta$. If we start with a lattice with a repeat length of F_m links, then after decimating m times we are left with a simple periodic lattice entirely composed of A-type links. $\sigma^{(m)}$, therefore, is the value of σ for a chain entirely composed of A-type links. For such a chain, every current I_n is related to its neighbors by Eq. (7), and, summing over all n, we find that

$$\sigma^{(m)} = i\omega \frac{N}{L} \frac{(h_\alpha^{(m)})^2}{\epsilon_\alpha^{(m)} - 2\gamma_A^{(m)}}, \tag{14}$$

where N is the total number of links in the chain. Combining Eqs. (13) and (14),

$$\sigma = \frac{i\omega}{L} \left(\frac{(h_\alpha^{(m)})^2 N}{\epsilon_\alpha^{(m)} - 2\gamma_A^{(m)}} + \sum_{l=0}^{m-1} N_\beta^{(l)} \frac{(h_\beta^{(l)})^2}{\epsilon_\beta^{(l)}} \right). \tag{15}$$

IV. RESULTS FOR THE CONDUCTIVITY

The first result to come out of Eq. (15) is that $\sigma = 0$ when $\omega = 0$. This is easily seen when one observes that all the quantities entering the bracket on the right-hand side of Eq. (15) are finite, even in the limit $\omega = 0$. Hence, in this limit, the factor of ω outside the brackets ensures that the conductivity will be zero. This is contrary to the prediction by Aldea and Dulea[6] that the conductivity would be finite as $\omega \to 0$.

Next, using Eq. (15) we have calculated the conductivity of chains formed by the infinite repetition of Fibonacci approximants up to about 100 000 links long for a variety of initial values of the variables. All the graphs we get are qualitatively the same, with two "resonances"—peaks in the imaginary part of σ—one in the region of $\omega = U_A$ and one at lower frequency. We find that the form of the curve has very little dependence on the period of repetition of the lattice. In Fig. 2 we display the hopping conductivity for a chain with a repeat length of 121 393 ($= F_{24}$) links and

$$U_A = 1, \quad U_B = 0.01, \quad d_A = 1, \quad d_B = 1.$$

The frequency ω is measured in units of U_A.

At very low frequencies $\mathrm{Re}\sigma \sim \omega^2$ and $\mathrm{Im}\sigma \sim \omega$. At very high frequencies $\mathrm{Re}\sigma$ is constant and $\mathrm{Im}\sigma \sim \omega^{-1}$. These results agree in form with the high- and low-frequency expansions performed by Aldea and Dulea,[6] except, again, we find that $\sigma \to 0$, rather than to a finite limit, as $\omega \to 0$.

It may at first appear odd that our results for the hopping conductivity of this system should yield an apparently smooth curve for σ against ω; the Miller-Abrahams equations on the Fibonacci chain bear a striking similarity to the equations used by earlier workers[2,3] to find the electron and phonon spectra of other models based upon the same chain, and yet those spectra display a complex, self-similar structure of which we see no sign in our results. The explanation lies in the appearance of the imaginary quantity $i\omega$ in the coefficients ϵ_α, ϵ_β, ϵ_γ. The corresponding quantity in the electron-phonon problem is real—it is the energy E of an electron, or the frequency squared ω^2 of a phonon.

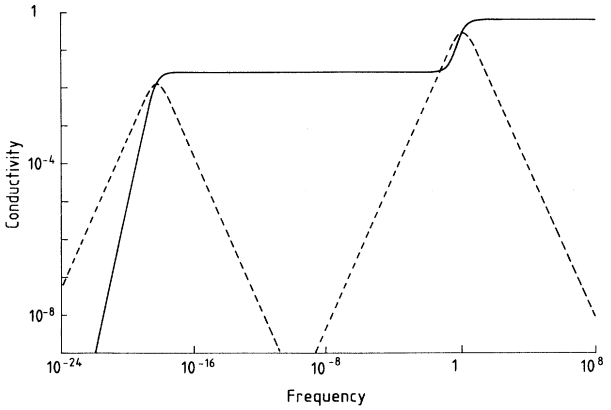

FIG. 2. Real (solid line) and imaginary (dashed line) parts of $\sigma(\omega)$ for a chain with a repeat length of 121 393 links. The sites are equally spaced and the hopping rates are $U_A = 1$ and $U_B = 0.01$. The frequency is in units of U_A.

If we rearrange the Miller-Abrahams equations thus,

$$\frac{i\omega}{U_n} I_n = I_{n-1} - 2I_n + I_{n+1} + i\omega E d_n,$$

it becomes apparent that except for the inhomogeneous term on the right-hand side the equations are nothing more than a finite difference version of the diffusion equation, with the diffusion coefficient varying along the lattice. In the phonon problem on the other hand, we have ω^2 instead of $i\omega$ on the left, so we get a wave equation. In order that there should be a finite current flowing throughout our infinite sample, we require of our solutions for the I_n that they neither decay nor grow exponentially along the lattice, which (still ignoring the inhomogeneous term) constricts them to being spatially constant. In the analogous phonon problem, however, the wave equation form allows the solutions to have spatially varying phase while still remaining finite, and it is solutions of this type that give rise to the complex spectra.

In reality, of course, the inhomogeneous term *is* present, and this does introduce some more interesting behavior in the conductivity. (After all, σ is not *totally* featureless.) But the crucial point is that oscillatory solutions for the I_n are not allowed, and these are the very solutions that produce the remarkable spectra seen in the earlier work.

There is another type of interesting behavior that we would expect to see in the conductivity, in its variation with the *length* of the sample for which it is calculated. The Landauer formula results of Sokoloff[5] and of Kohmoto and Sutherland[8] indicate that the conductivity should show oscillatory behavior with the length of the chain. It is one of the problems with the present model that we do not see this behavior. Of course, we do not expect to find it if we insist on making our calculations for an infinite lattice and performing a spatial average over the currents flowing in the lattice to get at the conductivity. However, it is a simple modification of our calculation to get the conductivity of a finite section of the chain by solving a finite set of Miller-Abrahams equations with the condition that the current flowing in one end of the chain should be the same as that flowing out the other end (equivalent to applying periodic boundary conditions to the infinite chain). However, since we believe interesting variations in the phases of the I_n as we move along the chain to be prohibited by the diffusion equation form, it is not surprising to find that the results so obtained for the conductivity are very similar to those for the infinite chain, and that no interesting variation with the length of the sample is revealed. This is a genuine shortfall of the model, and indicates the need for a more sophisticated calculation of the conductivity. Such a calculation would probably make use of either the Landauer formula,[9,5,8] or the full current-current correlation function, of which, as far as we are aware, no calculations have yet been made.

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