Conductance fluctuations in one-dimensional quasicrystals

S. Das Sarma and X. C. Xie
Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
(Received 27 July 1987)

We calculate the electronic resistance of a finite one-dimensional Fibonacci-sequence quasicrystal. We find that as a function of the electron energy (or, equivalently, the applied voltage) the electrical resistance of such quasicrystals shows strong fluctuations as resonant tunneling occurs through allowed energy states of the system. Evidence for power-law localization and self-similarity can be seen in the calculated transport properties and should be observable in artificially structured Fibonacci-sequence semiconductor superlattices.

There has been a great deal of recent theoretical interest[1-10] in the properties of one-dimensional (1D) quasiperiodic systems. While part of this interest is quite general, inspired originally by Aubry's work[11] on localization transition in 1D quasiperiodic systems, part of this work is certainly motivated by the recent discovery[12] of quasicrystals. A more significant development for 1D theories is the recent fabrication[13] by Merlin *et al.* of an artificial 1D "quasicrystal" employing a Fibonacci sequence of GaAs-$Al_xGa_{1-x}As$ multilayers. While there is still controversy[14] on whether the Al-Mn alloys (and other related three-dimensional "quasicrystalline" materials) discovered[12] by Shechtman *et al.* are actual quasicrystals or icosahedral glasses; the artificial 1D systems fabricated by Merlin *et al.* are, by construction, almost ideal (even though finite in size) quasiperiodic structures (albeit in 1D) on which one can test various theoretical ideas. Thus vibrational (phonons[15]), structural (x-ray structure factor), electronic (band structures), and collective properties (plasmons) of 1D quasicrystals have been calculated in the recent theoretical literature.[1-10]

Conspicuous in its absence, however, is a calculation of transport properties of 1D quasicrystals. In this paper we provide a direct numerical calculation, based on the Landauer formula,[16] of the conductance of finite 1D quasicrystals. Our numerical results will allow a direct comparison with experimental results if and when they are available.

Taking $\hbar=2m=1$, the Hamiltonian for an electron in the 1D quasicrystal is written as

$$-\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=E\psi(x)\ , \tag{1}$$

where $\psi(x)$ and E are the wave function and the energy of the electron, and $V(x)$ is the incommensurate potential due to the 1D quasicrystal. For $V(x)$ we choose the simplest Kronig-Penney–type model to write

$$V(x)=\sum_{n=1}^{N} q_n\delta(x-x_n)\ , \tag{2}$$

where q_n is the strength of the scattering potential located at $x=x_n$. The positions or sites x_n of the scatterers are distributed according to the Fibonacci sequence used[13] by Merlin *et al.* We choose two fundamental lengths a and b, and generate a Fibonacci sequence starting with a,ab, and $aab,aabab$, etc. The lth generation of the sequence is given simply by $S_l=\{S_{l-2},S_{l-1}\}$, with $S_0=a$ and $S_1=ab$. The lengths a and b determine the separations between the neighboring scatterers and the whole sequence determines where the scatterers are. Thus, the second generation (aab) has scatterers at $x_n=a$, $2a$, and $2a+b$. We should use at least two different scattering potential strengths q_n to accurately model the system of Ref. 13, but, in the spirit of the Kronig-Penney model (and also to keep the number of parameters a minimum) we choose $q_n=q=0.5$ for all the scatterers. Thus Fibonacci-sequence quasiperiodicity enters our theory only through the locations of the scatterers, their strengths being uniform in our model. We choose $a/b=\tau$ and $\frac{2}{3}$, where $\tau=(\sqrt{5}+1)/2$ is the golden mean—our results are qualitatively unchanged with any other (rational or irrational) choice of a/b since the basic quasiperiodicity of the model arises through the Fibonacci sequence. We want to emphasize that our scattering model is equivalent to the tight-binding model used by a number of authors to calculate the electronic band structure of this system. The scattering approach is, however, easier to implement in the numerical calculation of the conductance where one envisions electrons being injected into the system at the left and removed at the right after they tunnel through the potential barriers.

In calculating the transport coefficient we follow the Landauer approach[16] which is well suited for our purpose. For simplicity we use the single-channel Landauer formula[17] assuming ideal lead electrodes connected to the two ends of our superlattice. The system conductance is given by

$$G=\left[\frac{2e^2}{h}\right]\left[\frac{T}{1-T}\right]\ , \tag{3}$$

where T is the transmission coefficient through the whole quasicrystal. The resistance of the structure is given by

$$R = 1/G \ . \tag{4}$$

The transmission coefficient T is easy to obtain for a 1D system of δ-function scatterers by a repeated application of the transfer matrix M_i which relates the wave function $\psi_L^{(i)}$ on the left with the wave function $\psi_R^{(i)}$ on the right at the ith potential site,

$$\psi_R^{(i)} = M_i \psi_L^{(i)} \ . \tag{5}$$

Propagation of the electron from the jth site to the next site is given by the matrix $\bar{X}_j$,

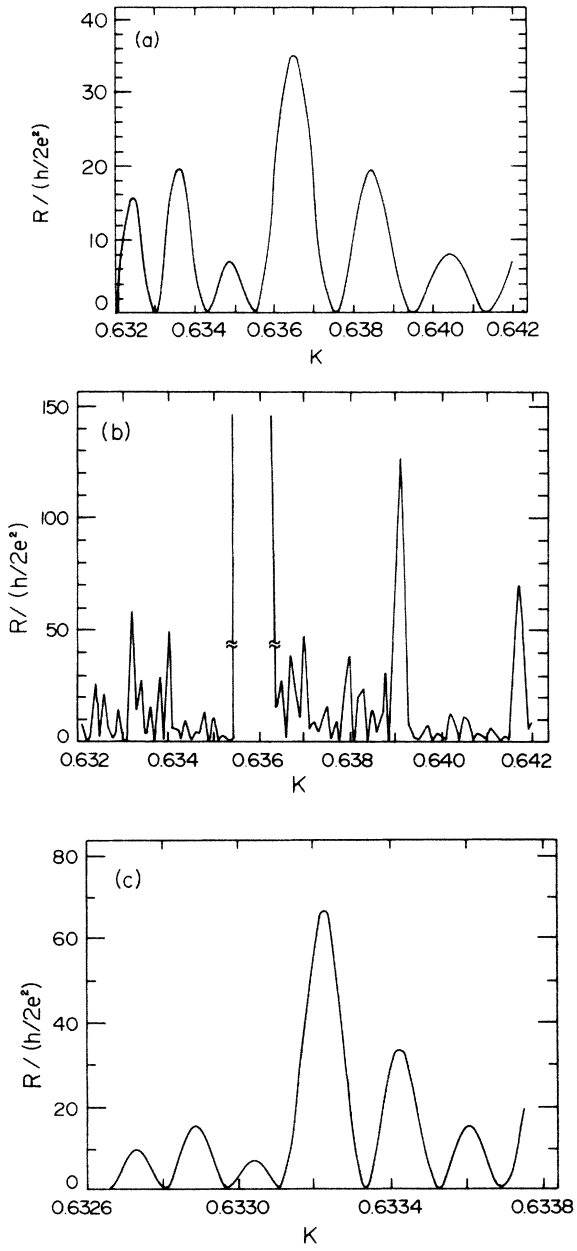

FIG. 1. Calculated resistance (R) as a function of $k = \sqrt{E}$ for (a) 12th and [(b) and (c)] 16th-generation Fibonacci superlattices with $a = 1.0$ and $b = 1.5$ as the two fundamental lengths. The self-similar structure can be clearly seen by comparing (a) and (c).

$$\bar{X}_j = \begin{bmatrix} e^{ikx_j} & 0 \\ 0 & e^{-ikx_j} \end{bmatrix} , \tag{6}$$

where $E = k^2$ is the energy of the electron. The total transfer matrix M for the system is given by

$$M = (\bar{X}_1 M_1)(\bar{X}_2 M_2)(\bar{X}_3 M_3) \cdots (\bar{X}_N M_N) \ . \tag{7}$$

Note that quasiperiodic, periodic, and random systems can be simulated in our model by taking the sites x_j's to be distributed quasiperiodically, periodically, and randomly, respectively.

It can be shown[17] that the transfer matrix M defined by Eq. (7) is related to the transmission coefficient by the relation

$$M^+ M = \begin{bmatrix} 1+2|r|^2/|t|^2 & 2r/t^2 \\ 2r^*/t^{*2} & 1+\dfrac{2|r|^2}{|t|^2} \end{bmatrix} , \tag{8}$$

where $|t|^2 = T$ is the transmission coefficient and $|r|^2 = (1-T)$ is the reflection coefficient. Thus, knowing the diagonal components of the transfer matrix is equivalent to knowing the (dimensionless) conductance or the resistance of the system [cf. Eqs. (3) and (4)].

We calculate the system resistance numerically by using Eqs. (1)–(8). All our conductance (resistance) is measured in units of $2e^2/h$ ($h/2e^2$). In Figs. 1(a) and 1(b) we show our calculated resistance as a function of $k = \sqrt{E}$ for 12th- and 16th-generation Fibonacci superlattices, respectively (with $a = 1.0$ and $b = 1.5$ as the two fundamental lengths). The self-similar structure of the resistance becomes obvious from Fig. 1(c) [by comparing with Fig. 1(a)], where we have blown up Fig. 1(b) around a small region of k values. In Fig. 2 we show our conductance results with $a = \tau$ and $b = 1$ for 12th-, 14th- and 16th-generation Fibonacci systems. Results in Figs. 1 and 2 look quite similar, indicating that the ratio a/b is not a significant parameter.

In Fig. 3 we study in more detail the self-similarity in the transport properties of a 16th-generation Fibonacci superlattice with $a = \tau$ and $b = 1$. We show our calculated conductance as a function of the electron momentum $k = \sqrt{E}$ in Figs. 3(a)–3(e) with progressively higher resolution. The resolutions Δk in k values are $\Delta k = 0.02$, 0.01, 0.002, 0.0005, and 0.0002, shown in Figs. 3(a)–3(e), respectively. Thus these results show self-similarity in the conductance up to a factor-of-100 magnification. In an ideal infinite Fibonacci quasicrystal, the spectrum of states is a Cantor set and the self-similarity exists to infinite resolution. In a real finite system, natural limits to this self-similarity are set by the finite system size and by inherent broadening effects from fluctuations, impurities, and finite temperature. The triplet structure of peaks seen in Figs. 3(a)–3(e) is a natural property of Fibonacci quasiperiodicity arising from the Cantor-set nature of the underlying spectrum. Our simulation, as shown in Figs. 3(a)–3(e), indicates

that this particular feature of the Cantor-set spectrum should show up in the experimentally measured transport properties of a Fibonacci superlattice.

The conductance (or, equivalently, the resistance) fluctuations seen in Figs. 1–3 can be understood as the physics of a finite Fibonacci superlattice, where, for a given system size, the eigenenergies form a set of sparse points (approaching a Cantor-set structure as the system size approaches infinity). As the electron energy equals one of these energy levels, there is enhanced resonant tunneling leading to high-conductance peaks. With increasing length of the quasicrystal (i.e., for higher generation Fibonacci superlattices) the spectrum becomes denser, leading to denser (i.e., "higher-frequency") conductance fluctuations as a function of electron energy. In Fig. 4 we study the systematic dependence of the average resistance $\bar{R}$ of a Fibonacci superlattice on its total length. The averaging has been done by calculating

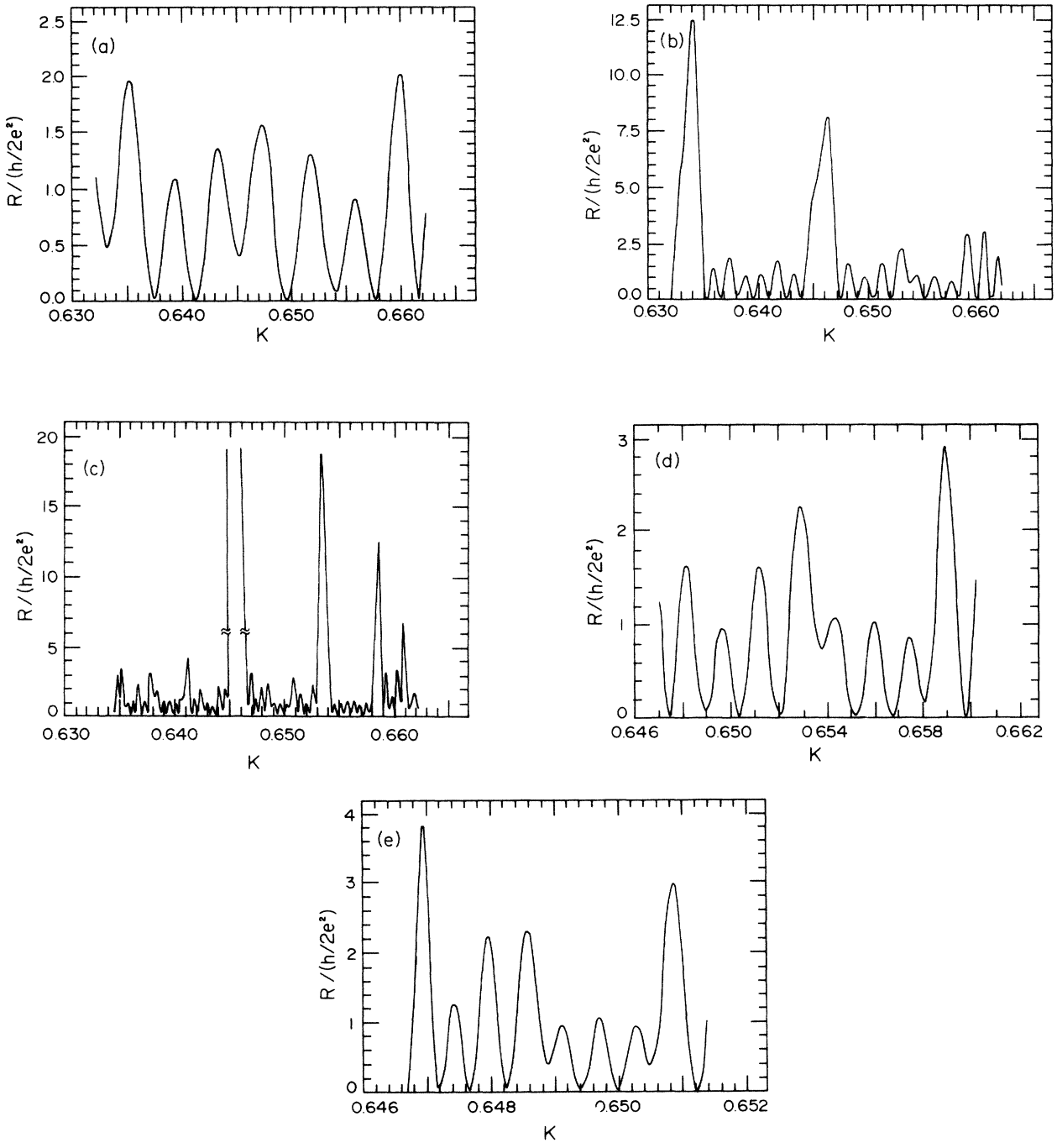

FIG. 2. Calculated resistance as a function of k for (a) 12th, (b) and (d) 14th, and [(c) and (e)] 16th-generation Fibonacci sequences with $a=\tau$, $b=1.0$. The self-similarity shows up in (a), (d), and (e).

$R(k)$ for each length between $k=0.9$ and 1.0, and then defining the average resistance on a k mesh with $\Delta k=0.005$. Thus, $\bar{R}=\frac{1}{21}\sum_{i=0}^{20}R_i(k_i)$ with $k_i=0.90+i(\Delta k)$. With other possible definitions of average resistance the result shown in Fig. 4 does not change qualitatively. The systematic increase of $\bar{R}$ with the length of the superlattice in a power-law fashion is consistent with our understanding of the power-law "localization" of the Fibonacci spectrum. Thus the finite conductance of a 1D Fibonacci quasicrystal is entirely due to its finite size. However, the increase in the resistance with the increase in the system length is rather weak (*not* exponential). This should be contrasted with the behavior of the resistance in the energy-gap regions of the spectrum where no resonant tunneling can take place and the resistance is exponentially large. It should be remarked that the Cantor-set spectrum of an ideal infinite Fibonacci quasicrystal has gaps everywhere.

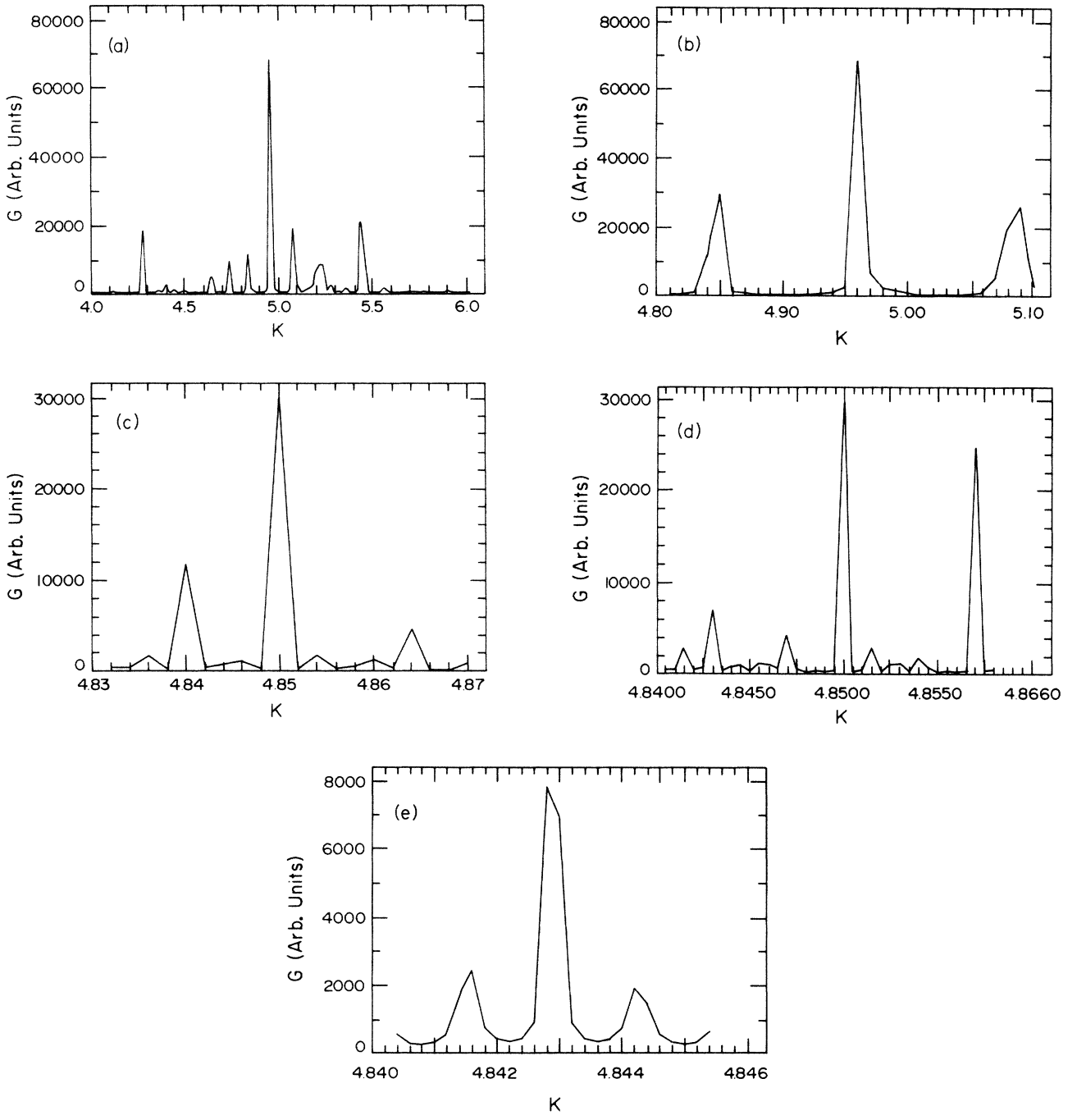

FIG. 3. Calculated conductance (G) for a 16th-generation Fibonacci sequence with $a=\tau$, $b=1.0$. Results are shown with different resolutions $\Delta k=0.02$ (a), 0.002 (c), 0.0005 (d), and 0.0002 (e).

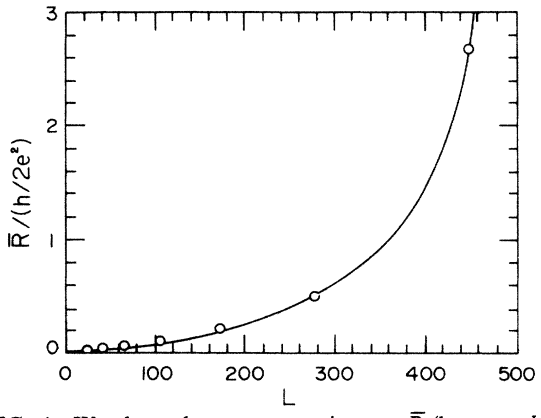

FIG. 4. We show the average resistance $\bar{R}$ (between $k=0.9$ and $k=1.0$) as a function of the total length L of the quasicrystal.

However, in real finite systems, lack of infinite resolution would allow one to see only the "large" gaps (larger than the inherent energy resolution of the system). Thus, the results shown in this paper indicate what transport properties of a real 1D quasicrystal, such as the one fabricated by Merlin *et al.*,[13] may look like.

Finally we consider the effects of departure from the ideal Fibonacci structure on the transport properties of our 1D quasicrystal. In any real situation, the fundamental widths a and b from which the Fibonacci superlattice has been constructed will vary somewhat from layer to layer, introducing random disorder into the quasicrystalline structure. In the ideal (and infinite) situation, introduction of any disorder will give rise to Anderson localization.[18] But in practical situations a small amount of random disorder will produce localization

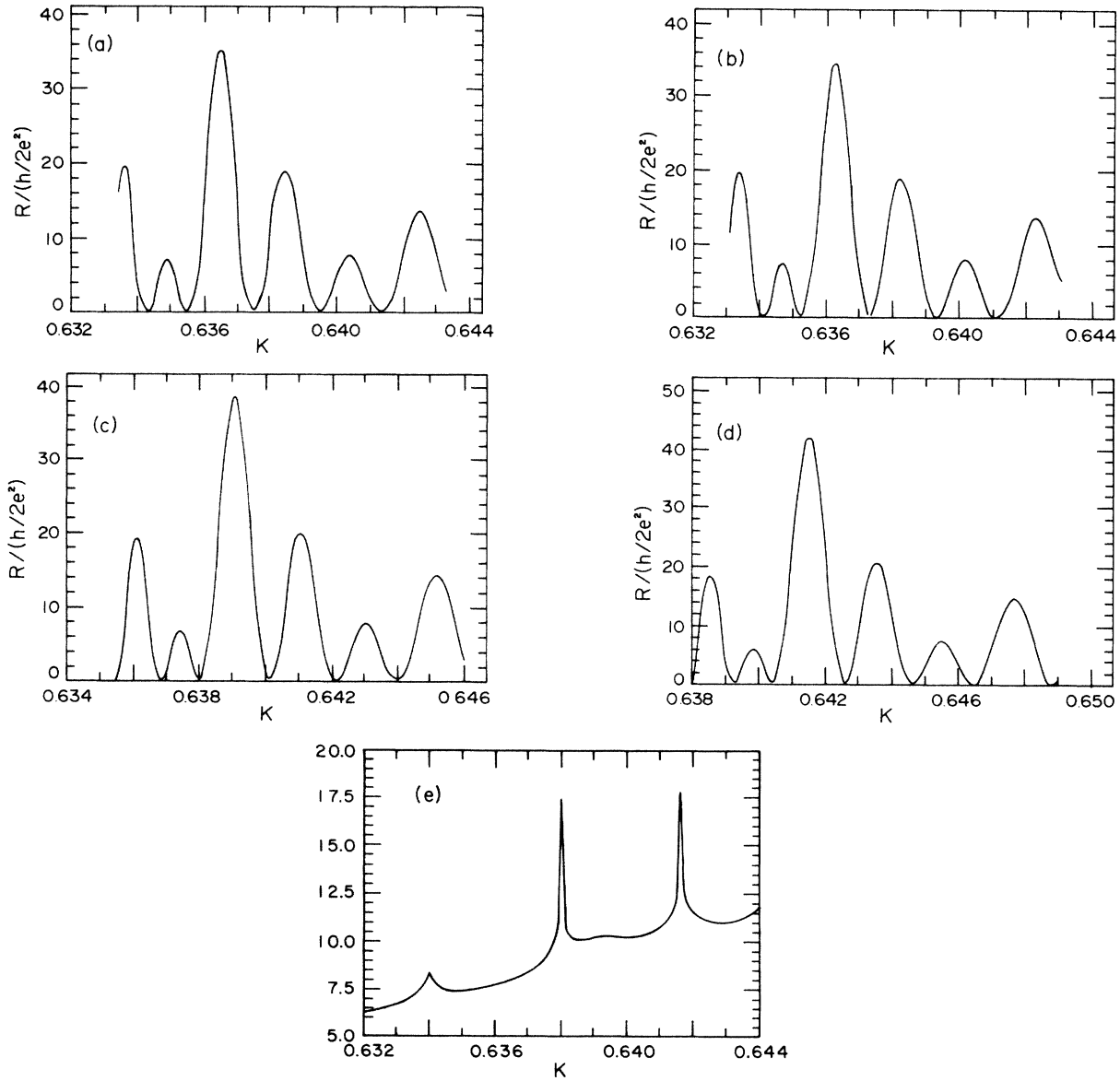

FIG. 5. (a) We show the resistance R as a function of k with $a=1.0$, $b=1.5$ for a 12th-generation Fibonacci superlattice. (b), (c), and (d) are the same as (a), but with width fluctuations up to 1%, 5%, and 10%, respectively. (e) We show the localization length ξ as a function of k for random order of a and b.

lengths substantially larger than the system size, thus not affecting the quasicrystalline physics being studied here. In fact, artificially structured 1D quasicrystals based on semiconductor superlattices allow one to study the interplay of quasiperiodicity and disorder in a controlled fashion.

In Figs. 5(a)–5(d) we show the effect of disorder on the transport properties of a 12th-generation Fibonacci superlattice. We introduce disorder by making the widths a and b vary randomly from layer to layer in the Fibonacci structure. Thus we take $a=a_0+\Delta a$ and $b=b_0+\Delta b$, with $a_0=1.0$, $b=1.5$, as in Figs. 1 and 4 (where $\Delta a=\Delta b=0$). The width fluctuations Δa and Δb are taken to be 1%, 5%, and 10%, as shown in Figs. 5(b)–5(d), respectively, whereas in Fig. 5(a) we show the results [same as Fig. 1(a)] for the ideal system ($\Delta a=\Delta b=0$). It is obvious from these figures that even for width fluctuations as large as 10%, the transport properties of the Fibonacci superlattice remain qualitatively unchanged. There is only a small overall shift in the curves for various disorder compared with the ideal situation shown in Fig. 5(a). This shows that if vertical tunneling transport experiments[19] can be carried out in 1D quasicrystals,[13] the conductance fluctuations discussed in this paper should be experimentally observable in real structures in spite of the existence of a small amount of disorder. If we keep the respective number of fundamental lengths a and b the same as in Fig. 5(a), but put them in a random order, we find resistance $R\sim e^{L/\xi}$ as expected. In Fig. 5(e) we plot localization length ξ as a function of k.

In conclusion, we have calculated numerically the transport properties of a 1D Fibonacci superlattice using the Landauer approach. We find considerable conductance fluctuations as a function of the energy of the tunneling electron. These fluctuations reflect the Cantor-set spectrum of the system and are self-similar in nature. We study the length dependence of the system resistance and find a behavior consistent with a power-law localization. Our calculated conductance fluctuations are fairly insensitive to the existence of a small ($\lesssim 10\%$) amount of disorder in the system. A fairly large number of experimental papers[19] have appeared in the recent literature reporting the observation of Bloch transport in a *periodic* superlattice (along the superlattice direction) using a variety of tunneling techniques. We strongly urge that such experiments be performed on a 1D Fibonacci superlattice[13] to directly study the conductance fluctuations predicted in this paper.

This work is supported by the U.S. Army Research Office (ARO), the U.S. Office of Naval Research (ONR), and the U.S. Department of Defense (DOD). Computer time has been supplied by the University of Maryland Computing Center.

[1]B. Simon, Adv. Appl. Math. **3**, 463 (1982), and references therein.

[2]S. Ostlund and R. Pandit, Phys. Rev. B **29**, 1394 (1984).

[3]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983); M. Kohmoto, B. Sutherland, and C. Tang, Phys. Rev. B **35**, 1020 (1986).

[4]R. K. Zia and W. J. Dallas, J. Phys. A **18**, L341 (1985).

[5]J. P. Lu, T. Odagaki, and J. L. Birman, Phys. Rev. B **33**, 4809 (1986).

[6]F. Nori and J. Rodriquez, Phys. Rev. B **34**, 2207 (1986); Q. Niu and F. Nori, Phys. Rev. Lett. **57**, 2057 (1986).

[7]J. M. Luck and D. Petritis, J. Stat. Phys. **42**, 298 (1986).

[8]J. B. Sokoloff, Phys. Rev. B **23**, 6422 (1981); A. D. Zdetsis, C. M. Soukolis, and E. N. Economou, *ibid.* **33**, 4936 (1986); D. R. Grempel, S. Fishman, and R. E. Prange, Phys. Rev. Lett. **49**, 833 (1982).

[9]S. Das Sarma, A. Kobayashi, and R. E. Prange, Phys. Rev. Lett. **56**, 1280 (1986); Phys. Rev. B **34**, 5309 (1986).

[10]P. Hawrylak and J. J. Quinn, Phys. Rev. Lett. **57**, 380 (1986).

[11]S. Aubry, *Annals of the Israel Physical Society,* edited by C. G. Kuper (Hilger, Bristol, 1979), Vol. 3, p. 133.

[12]D. Shechtman, I. Bloch, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984); D. Levine and P. J. Steinhardt, *ibid.* **53**, 2477 (1984).

[13]R. Merlin, K. Bajema, R. Clarke, F. Y. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. **55**, 1768 (1985); J. Todd, R. Merlin, R. Clarke, K. M. Mohanty, and J. D. Axe, *ibid.* **57**, 1157 (1986).

[14]P. W. Stephens and A. I. Goldman, Phys. Rev. Lett. **56**, 1168 (1986).

[15]M. W. C. Dharma-wardana, A. H. MacDonald, D. J. Lockwood, J. M. Baribeau, and D. C. Houghton, Phys. Rev. Lett. **58**, 1761 (1987).

[16]R. Landauer, IBM J. Res. Dev. **1**, 223 (1957); Philos. Mag. **21**, 863 (1970); P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B **22**, 3519 (1980).

[17]B. S. Adereck and E. Abrahams, *Physics in One Dimension,* edited by J. Bernasconi and T. Schnieder (Springer-Verlag, New York, 1981).

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

[19]B. Deveaud *et al.*, Phys. Rev. Lett. **58**, 2582 (1987); F. Capasso *et al.*, *ibid.* **55**, 1152 (1985); R. A. Davies *et al.*, *ibid.* **55**, 1114 (1985); J. F. Palmier *et al.*, Appl. Phys. Lett. **49**, 1260 (1986); D. V. Lang *et al.*, *ibid.* **49**, 812 (1986); A. Nakamura *et al.*, Phys. Rev. B **34**, 9010 (1986); G. Belle *et al.*, Solid State Commun. **56**, 65 (1985); T. Duffield *et al.*, Phys. Rev. Lett. **56**, 2724 (1986).