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Band structure and localization in incommensurate lattice potentials

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A metal-insulator transition was found by Aubry in a one-dimensional tight-binding model containing a modulation potential incommensurate with the crystal lattice. In this article the extended bandlike states that occur in the metallic regime are studied using a quasiclassical approach. Near the metal-insulator transition the bands contain a hierarchy of gaps of ever decreasing magnitude. Although there is in principle a gap at every energy, since most gaps are negligible, the system is still expected to behave like a metal. In the insulating regime the wave functions were found to be exponentially localized with a localization length which approaches infinity at the metal-insulator transition. Possible experimental consequences of the predicted spectrum are discussed.

I. INTRODUCTION

Crystalline solids with two incommensurate periodic potentials form a class of solid intermediate between crystalline and disordered. Unlike disordered solids for which all single-particle states are localized in one dimension, and periodic solids for which all states are extended, these solids possess a metal-to-insulator transition in one dimension in which the system switches from all states extended to all states localized, as a function of the strength of the periodice modulation potential.[1] Examples of solids with incommensurate periodic potentials are crystals with charge- and spin-density waves,[2] ionic conductors,[3] crystals with artificially produced superlattices,[4] and certain alloys.[5] Aubry has claimed that the metal-insulator transition represents a transition in which the analyticity of the wave function is broken.[1] Azbel has discussed the spectrum of such systems using quasiclassical methods valid for very-long-period modulations.[6] The present author has shown that such methods can be used even for short-period incommensurate modulations.[7] These methods always show a changeover from a state in which all the classical trajectories are localized to one in which some of them are extended at the point of the insulator-metal transition. One would then expect that tunneling between the localized trajectories would broaden then into bands of extended states, implying that all states are extended.[8] Since the quasiclassical methods depend on replacing the difference equation by a differential equation, however, a metal-insulator transition could still occur if there were a break in analyticity of the wave functions, in the sense that the solution to the difference equation ψ_n cannot be continued to noninteger values of n in the insulating regime as claimed by Aubry.[1] In the present article Aubry's claim is substantiated. By using quasiclassical methods on the metallic side and perturbation theory on the insulating side, it is possible to study the band structure and the form of the wave functions, and thus give a physical picture of the metal-insulator transition and to predict certain experimental consequences. The picture that emerges is a transition from extended but narrow bandlike states to exponentially localized states. The energy spectrum switches from a spectrum of narrow bands separated by gaps on the metallic side to a spectrum of discrete energy levels on the insulating side.

II. THE METAL-INSULATOR TRANSITION CAUSED BY INCOMMENSURABILITY

Aubry[1] has shown, using a formula from Thouless,[9] that a one-dimensional tight-binding model with a sinusoidal modulation potential incommensurate with the lattice will undergo a metal-insulator transition when the modulation potential strength is equal to the bandwidth. The model that he considered is

$$t(\psi_{n+1}+\psi_{n-1})+V_0\cos(Qan+h)\psi_n=E\psi_n\,, \tag{1}$$

where t is the hopping matrix element, V_0 is the modulation potential strength, h is a phase factor, a is the lattice constant, and Q is the wave vector of the modulation. The wave function is defined by

$$\Psi(x)=\sum_n \psi_n\varphi(x-na)\,, \tag{2}$$

where $\varphi(x-na)$ is an atomic or Wannier function centered about site na. In this section, Aubry's results will be derived using a quasiclassical approach and perturbation theory. The quasiclassical method allows one to study the nature of the band structure in the metallic regime and the perturbational approach allows one to study the wave function in the insulating regime.

First, let us consider the metallic regime which

occurs when $V_0 < 2t$. Consider rational Q values [(i.e., $Q = (2\pi/a)(L/M)$, where L and M are integers]. Equation (1) can then be written as $M \times M$ almost tridiagonal matrix equation, i.e., an equation of the form[1]

$$\sum_{m'} \mathcal{H}_{mm'} f_{m'} = E f_m , \tag{3}$$

where

$$\mathcal{H}_{mm'} = 2t \cos[(k + mQ)a]\delta_{mm'} + \frac{V_0}{2}(\delta_{m,m'+1} + \delta_{m',m+1}) \tag{4}$$

for m and $m' \neq M$, and $\mathcal{H}_{0,M} = \mathcal{H}^*_{M,0} = (V_0/2)e^{iMh}$, where

$$\psi_n = e^{ikna} \sum_m f_m e^{iQmna} . \tag{5}$$

The secular determinant for Eq. (3) is easily shown to have the form[10]

$$\prod_{j=1}^{M} [E - E_j(k)] + \left(\frac{V_0}{2}\right)^M (1 - \cos Mh) = 0 , \tag{6}$$

where $E_j(k)$ are the eigenvalues for $h = 0$. Clearly for $V_0 \ll$ the bandwidth, the dependence of each band on the phase h is of the form

$$E = E_j(k) + O\left(\frac{V_0}{2t}\right)^M (1 - \cos Mh) . \tag{7}$$

Hence, in the incommensurate (i.e., $M \to \infty$) limit the band structure becomes independent of the phase. This is always the case if the solution to Eq. (1) can be analytically continued to noninteger values of n, since in such a case it is easily seen that if $\psi(n)$ is the solution for phase $h = 0$, $\psi[n + (h/Q)]$ is the solution for the same energy of Eq. (1) with phase h.[1]

It will now be shown that the band structure remains independent of phase for all $V_0 < 2t$, but that this behavior breaks down for $V_0 > 2t$. The calculation will be performed by recognizing that the self-energy S_n for the Green's function for Eq. (1), G_{nn}, can be written as[11]

$$S_n = \cfrac{t^2}{E - V_0 \cos Q(n+1)a - \cfrac{t^2}{E - V_0 \cos Q(n+2)a - \cfrac{t^2}{E_-}}} + \cfrac{t^2}{E - V_0 \cos Q(n-1)a - \cfrac{t^2}{E - V_0 \cos Q(n-2)a - \cfrac{t^2}{E_-}}} \cdot \tag{8}$$

If Q of the form $(2\pi/a)(L/M)$, the continued fractions are periodice (i.e., they repeat after M terms). If $X_\pm$ represents each of the continued fractions, it can be shown that[12]

$$X_\pm = \frac{P_M}{Q_M} , \tag{9}$$

where

$$P_M = (E - V_0 \cos QMa - X_\pm)P_{M-1} - t^2 P_{M-2} , \tag{10a}$$

$$Q_M = (E - V_0 \cos QMa - X_\pm)Q_{M-1} - t^2 Q_{M-2} . \tag{10b}$$

Equations (9) and (10) combined result in a quadratic equation for $X_\pm$. P_n and Q_n can be found by iterating difference equations.[12] If the solution is complex there is an extended state at energy E; if it is real there is a localized state. This method was used to search for the existence of bands of extended states. The results are shown in Fig. 1. As can be seen, the band structure becomes independent of the phase for $V_0 < 2t$ as M increases, but not for $V_0 > 2t$. Thus, from the arguments in the previous paragraph we conclude that ψ_n can only be analytic for $V_0 < 2t$. This is the analyticity-breaking transition predicted by Aubry.[1] Physically, it represents a breaking of translational symmetry in this problem.

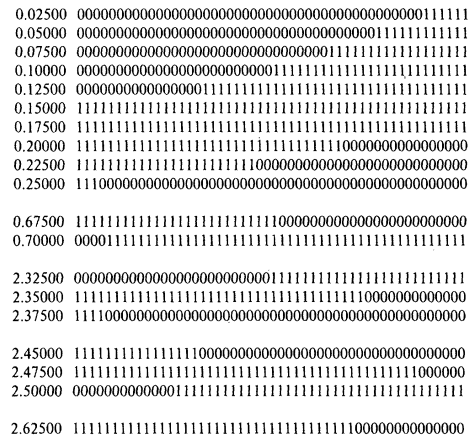
In Ref. 7 it was proposed that since Q could always be approximated by a high-order commensurate wave vector, we could use a quasiclassical approach to solve Eq. (1) to any desired degree of approximation. In this approach we write $Q = Q_0 + q$, where Q_0 is a high-order commensurate approximation to Q and q is the correction. Since $qa \ll 1$, we may, to first approximation, diagonalize Eq. (1) treating qan as a constant. The resulting phase trajectories $E_\alpha(k, qna) = E$, where E_α is the energy in the αth band, are the starting points for a WKB approximation in which q plays the role of $\hbar$[6,7] to treat the corrections due to the fact that qna is actually a variable and not a constant phase. The starting point for the WKB method is to replace Eq. (1) with a differential equation by using the relationship

$$\psi_{n\pm1} = \exp\left(\pm \frac{d}{dn}\right)\psi_n . \tag{11}$$

This procedure is only valid if ψ_n is an analytic function of n. Thus, from what was said in the previous paragraph it may be concluded that these methods are only valid for $V_0 < 2t$, and thus, they cannot allow us to conclude anything about the localization which occurs when $V_0 > 2t$. For $V_0 < 2t$, however, these methods allow us to draw a very important conclusion regarding the electronic structure. As seen in Figs. 1 and 2, if we take the phase to be qna, the "classical" trajectories are extended for $V_0 < 2t$. By approximating Q by a sufficiently high-order commensurate Q_0, q may be made arbitrarily small. The WKB method

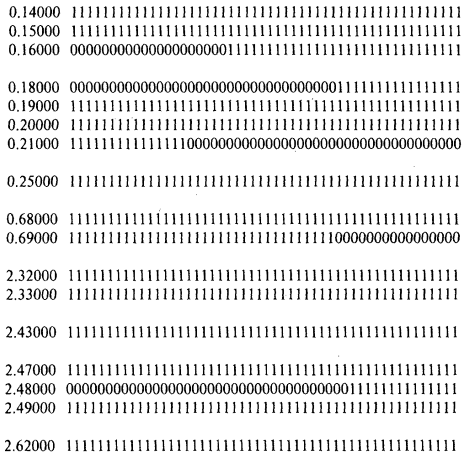
(a)

$h = 0$ to π/M in units of $2\pi/(100M)$



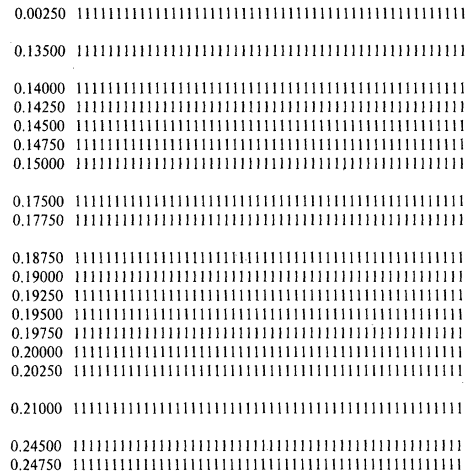
(b)

$h = 0$ to π/M in units of $2\pi/(100M)$



(c)

$h = 0$ to π/M in units of $2\pi/(100M)$



(d)

$h = 0$ to π/M in units of $2\pi/(100M)$

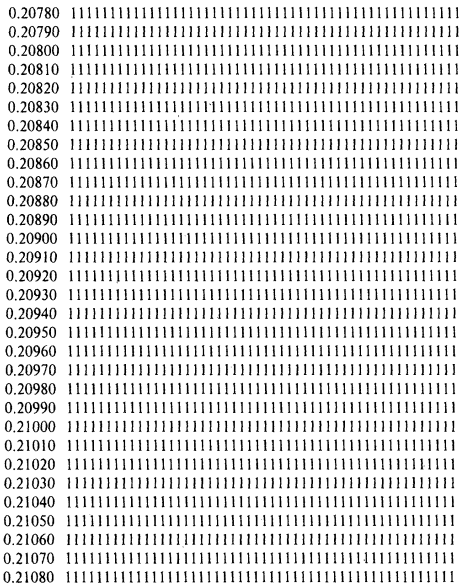


FIG. 1. Allowed bands as a function of phase h for h going from 0 to π/M for $V_0 = 1.9t$. The ones represent bands of extended states and the zeros are regions where no states exist. $Q/2\pi = \frac{3}{10}$ in (a), $\frac{10}{33}$ in (b), $\frac{33}{109}$ in (c). These values are obtained by keeping successive terms in the continued fraction expansion of

$$Q/2\pi = (\sqrt{13} - 3)/2 = \cfrac{1}{3 + \cfrac{1}{3 + \cfrac{1}{3 + \ddots}}} \quad .$$

In (d), a small range of energy for $Q/2\pi = \frac{33}{109}$ is looked at in more detail. The band structure becomes independent of h as $Q/2\pi$ is approximated by ratios of larger integers. Also to be noted is that no new gaps are introduced in the centers of the wider bands as $Q/2\pi$ is approximated by ratios of larger integers.

(a)

$h = 0$ to π/M in units of $2\pi/(100M)$

```
0.02500 00000000000000000000000000000000000000000000011111
0.05000 00000000000000000000000000000000000000000001111111
0.07500 00000000000000000000000000000000000000011111111111
0.10000 00000000000000000000000000000000111111111111111111
0.12500 00000000000000000000000000011111111111111111111111
0.15000 00000000000000000000011111111111111111111111111111
0.17500 00000000000000011111111111111111111100000000000000
0.20000 11111111111111111111111111110000000000000000000000
0.22500 11111111111111111111000000000000000000000000000000
0.25000 11111111111000000000000000000000000000000000000000

0.70000 11111111110000000000000000000000000000000000000000
0.72500 00000000011111111111111111111100000000000000000000
0.75000 00000000000000000000000000000000011111111111111111

2.45000 00000000000000000000000011111111111111111111111111
2.47500 11111111111111111111100000000000000000000000000000

2.57500 11111111110000000000000000000000000000000000000000
2.60000 11111111111111111111111100000000000000000000000000
2.62500 00000000000000000000011111111111111111111111111111
2.65000 00000000000000000000000000000000000000011111111111

2.75000 00000000000000000000111111111111111111111111111111
```

(b)

$h = 0$ to π/M in units of $2\pi/(100M)$

```
0.15000 00000000000011111111000000000000000000000000000000
0.16000 00000000000000000000000000011111111000000000000000
0.17000 00000000000000000000000000000000000000001111111111

0.19000 00000000000000000000000000000000000000000011111111
0.20000 00000000000000000000000000001111111100000000000000
0.21000 00000000000000000011111100000000000000000000000000
0.22000 11111110000000000000000000000000000000000000000000

0.26000 00000000000000000000001111110000000000000000000000

0.73000 00000000000000000000000000001111111100000000000000
0.74000 00000000000000000000011111110000000000000000000000

2.44000 11111111110000000000000000000000000000000000000000
2.45000 00000000000000000001111110000000000000000000000000

2.59000 00000000000111111110000000000000000000000000000000
2.60000 00000000000000000000000000000000000001111111111111
2.61000 00000000000000000000000000000000000011111111111111
2.62000 11111111111111000000000000000000000000000000000000

2.76000 00000000000000000000000000000000000011111111111111
```

(c)

$h = 0$ to π/M in units of $2\pi/(100M)$

```
0.25505 11111111111000000000000000000000000000000000000000
0.25510 11111111111000000000000000000000000000000000000000
0.25515 11111111111000000000000000000000000000000000000000
0.25520 11111111111000000000000000000000000000000000000000
0.25525 11111111111000000000000000000000000000000000000000
0.25530 11111111111000000000000000000000000000000000000000
0.25535 11111111111000000000000000000000000000000000000000
0.25540 11111111111000000000000000000000000000000000000000
0.25545 11111111111000000000000000000000000000000000000000
0.25550 11111111111000000000000000000000000000000000000000
0.25555 11111111111000000000000000000000000000000000000000
0.25560 11111111111000000000000000000000000000000000000000
0.25565 11111111111000000000000000000000000000000000000000
0.25570 11111111111000000000000000000000000000000000000000
0.25575 11111111111000000000000000000000000000000000000000
0.25580 11111111111000000000000000000000000000000000000000
0.25585 11111111111000000000000000000000000000000000000000
0.25590 11111111111000000000000000000000000000000000000000
0.25595 00111111111111000000000000000000000000000000000000
0.25600 00011111111111000000000000000000000000000000000000
0.25605 00011111111111000000000000000000000000000000000000
0.25610 00001111111111000000000000000000000000000000000000
0.25615 00001111111111000000000000000000000000000000000000
0.25620 00000111111111000000000000000000000000000000000000
0.25625 00000111111111000000000000000000000000000000000000
0.25630 00000111111111000000000000000000000000000000000000
0.25635 00000111111111000000000000000000000000000000000000
0.25640 00000111111111000000000000000000000000000000000000
0.25645 00000011111111000000000000000000000000000000000000
0.25650 00000011111111000000000000000000000000000000000000
0.25655 00000001111111100000000000000000000000000000000000
0.25660 00000001111111100000000000000000000000000000000000
0.25665 00000001111111100000000000000000000000000000000000
0.25670 00000001111111100000000000000000000000000000000000
0.25675 00000000111111110000000000000000000000000000000000
0.25680 00000000111111110000000000000000000000000000000000
0.25685 00000000111111110000000000000000000000000000000000
0.25690 00000000011111111000000000000000000000000000000000
0.25695 00000000011111111000000000000000000000000000000000
0.25700 00000000011111111000000000000000000000000000000000
0.25705 00000000011111111000000000000000000000000000000000
0.25710 00000000011111111000000000000000000000000000000000
0.25715 00000000011111111000000000000000000000000000000000
0.25720 00000000001111111100000000000000000000000000000000
0.25725 00000000001111111100000000000000000000000000000000
0.25730 00000000001111111100000000000000000000000000000000
0.25735 00000000000111111110000000000000000000000000000000
0.25740 00000000000111111110000000000000000000000000000000
0.25745 00000000000111111110000000000000000000000000000000
0.25750 00000000000011111111000000000000000000000000000000
0.25755 00000000000011111111000000000000000000000000000000
0.25760 00000000000011111111000000000000000000000000000000
```

(d)

$h = 0$ to π/M in units of $2\pi/(100M)$

```
0.20200 00000000000010000000000000000000000000000000000000

0.20500 10000000000000000000000000000000000000000000000000
0.20600 01000000000000000000000000000000000000000000000000

0.21100 00000000000000000000000010000000000000000000000000
0.21200 00000000000000000000000000010000000000000000000000

0.21800 00000000000000000000000000000000000000000000000100
```

(e)

$h = 0$ to π/M in units of $2\pi/(100M)$

```
0.20130 00000000000000001000000000000000000000000000000000

0.20150 00000000000000010000000000000000000000000000000000

0.20200 00000000000010000000000000000000000000000000000000

0.20220 00000000000010000000000000000000000000000000000000

0.20270 00000000010000000000000000000000000000000000000000

0.20290 00000000010000000000000000000000000000000000000000
```

FIG. 2. Allowed states are shown as a function of phase h for h going from 0 to π/M for $V_0 = 2.1t$ for $Q/2\pi = \frac{3}{10}$ in (a), $\frac{10}{33}$ in (b), and $\frac{33}{109}$ in (d). In (c) and (e) a more detailed view of the energy levels shown in (b) and (d), respectively, is shown. It should be noted that the states are never independent of phase.

may now be applied to the "classical trajectories." The problem of using the WKB method to treat open phase trajectories has already been studied by Zilberman[13] for the problem of an electron in a magnetic field, and the results may be taken over completely for the present problem. The WKB calculation of Zilberman shows that new gaps are introduced in the "classical" extended-state bands but as we move into the center of the bands the gaps decrease in magnitude as $e^{-cE/q}$, where c is a constant and E is the energy measured from the "classical" band edge. Thus, for small q the gaps become negligible as we move into centers of the bands. This effect may be verified by examining the "classical phase trajectories," shown in Fig. 1. Because almost every wave vector is a reciprocal-lattice vector (because all sums and differences of the reciprocal-lattice vectors of both periodic potentials are reciprocal-lattice vectors), there should be band gaps almost everywhere. Most of the gaps, however, are negligibly small. Thus, although in theory one might expect the bands of an incommensurate system to become completely fragmented into negligibly narrow bands, the reverse is actually true. Each band contains a hierarchy of gaps that become negligibly small as one gets into the centers of the bands. When V_0 approaches $2t$, although the bands get broken up into narrower and narrower sub-bands, the sub-bands do not really become fragmented further into subands of neglibible width because the gaps that occur away from the edges of the "classical" bands have negligible widths and as such are insignificant. (They are insignificant in the sense that electrons Zener tunnel through them even in an infinitesimal electric field.)

Since we have seen that for $V_0 > 2t$ the WKB method cannot be used, the wave functions will now be studied using perturbation theory valid for $V_0 > 2t$. For $t = 0$, each Wannier function is obviously an eigenstate and the energy of the Wannier function on site n is $V_0 \cos Qna$, which gives a continuum of discrete states. As t is increased from zero, we expect each of these Wannier functions to mix in such a way that the resulting state decays exponentially as we move away from the site around which it is localized. Let us look for a state localized about site n_0. Then, if we assume $\psi_{n_0} = 1$, it can easily be shown by iterating Eq. (1) that for $n > n_0$ (upper sign) and $n < n_0$ (lower sign),

$$\psi_n = \frac{t^{(n-n_0)}}{\epsilon_1\epsilon_2\cdots\epsilon_n} \frac{1}{\left(1-\frac{t^2}{\epsilon_1\epsilon_2}\right)\left(1-\frac{t^2}{\epsilon_2\epsilon_3\left(1-\frac{t^2}{\epsilon_1\epsilon_2}\right)}\right)\cdots\left(1-\frac{t^2}{\epsilon_n\epsilon_{n-1}\left(1-\frac{t^2}{\epsilon_{n-1}\epsilon_{n-2}}\right)\ddots}\right)\left(\frac{\frac{t}{\epsilon_n}\psi_{n+1}}{1-\frac{t^2}{\epsilon_n\epsilon_{n-1}\left(1-\frac{t^2}{\epsilon_{n-1}\epsilon_{n-2}}\right)\ddots}}\right)}, \tag{12}$$

where $\epsilon_n = E - V_0\cos[Q(n \pm n_0) + h]$. It is easily shown that the second term is of order $(t/V_0)^2$ smaller than the first term in Eq. (12). The continued fractions in (12) do not affect the value of ψ_n significantly. Thus, if E is not equal to a value which makes one of the continued fractions vanish, the first term in Eq. (12) may be replaced by its geometric mean, $(2t/V_0)^{(n-n_0)}$. Thus, we conclude that ψ_n decays with exponent γ given by

$$\gamma = \ln\left(\frac{V_0}{2t}\right) \tag{13}$$

in agreement with Aubry.[1] The decay length $1/\gamma$ becomes infinitely large as $V_0 \to 2t$. For incommensurate Q, the above procedure is valid because for most values of E the denominators will not vanish. Such terms of successively higher order were calculated numerically to verify this conclusion.[14] The energy eigenvalues are calculated by using the difference equation for ψ_{n_0}, which becomes for $\psi_{n_0} = 1$,

$$E = V_0\cos(Qn_0 + h) + (\psi_{n_0+1} + \psi_{n_0-1}) . \tag{14}$$

Substituting for $\psi_{\pm 1}$ from Eq. (12) we obtain a perturbation theory for E.

Incidentally, for $V_0 < 2t$, Aubry[1] has shown that Eq. (1) may be transformed using

$$\psi_n = e^{ikn}\sum_{m=-\infty}^{\infty} f_m e^{i(Qn+h)m} \tag{15}$$

to the equation

$$t'(f_{m+1}+f_{m-1})+V_0'\cos(Qm+k)f_m=Ef_m, \tag{16}$$

where $V_0'=4t$, and $t'=V_0$. Then, by making the substitutions $f_m \rightleftharpoons \psi_n$, $V_0' \rightleftharpoons V_0$, $t' \rightleftharpoons t$, and $k \rightleftharpoons h$, Eqs. (12)–(14) may be taken over to treat the f's, which are localized in k space in this regime. In the lowest few orders this is recognized as the nearly-free-electron model.

The nth-order term in the perturbation theory for the energy obtained by substituting Eq. (12) into Eq. (14) is of the form

$$\frac{t^{n+2}}{\epsilon_1\cdots\epsilon_{n-2}\epsilon_{n-1}^2}\frac{1}{\left(1-\frac{t^2}{\epsilon_1\epsilon_2}\right)\left(1-\frac{t^2}{\frac{\epsilon_3\epsilon_2}{1-\frac{t^2}{\epsilon_1\epsilon_2}}}\right)\cdots\left(1-\frac{t^2}{\frac{\epsilon_{n-1}\epsilon_{n-2}}{1-\frac{t^2}{\frac{\epsilon_{n-2}\epsilon_{n-3}}{1-\ddots}}}}\right)^2\left(1-\frac{t^2}{\frac{\epsilon_n\epsilon_{n-1}}{1-\frac{t^2}{\frac{\epsilon_{n-1}\epsilon_{n-2}}{1-\ddots}}}}\right)}. \tag{17}$$

This term has a simple pole when one of the last two contined fractions in the denominator vanishes (which occurs in the vicinity of $\epsilon_n=0$ for small t). The dependence of the perturbation theory represented by Eq. (14) on E is illustrated qualitatively in Fig. 3. Also illustrated is an illustrative straight line to represent $E-V_0\cos(Qn+h)$. Each intersection of these curves represents a state. When h is such that two successive solutions have minimum separation, the energy difference between these states represents the energy gap in the bands of E versus h. Since the pole which occurs in the vicinity of $\epsilon_n=0$ occurs in a term of order $(2t/V_0)^n$, we conclude that the residue is of this order. (Remember that when a denominator is not close to vanishing, we may approximate it by its geometric mean.) Thus, the corresponding gap will be of order $(2t/V_0)^{n/2}$. Note that since the actual solution for the energy will lie away from any poles in the perturbation theory, the perturbation theory for the wave function in Eq. (12) will be well behaved at the eigenvalue, and hence, the arguments given below Eq. (12) are still correct.

When the same arguments are applied to the case $V_0<2t$ using Eq. (15) and (16), we conclude that although there exists a gap at every energy, most of the gaps are high-order gaps which come about because of poles in very-high-order terms in perturbation theory. Since these poles have negligible residues, most of the high-order gaps are negligible, although as V_0 approaches $2t$, more and more of the gaps become important. This conclusion agrees with the argument given earlier in this section, based on quasiclassical methods. The advantage of the method based on perturbation theory, however, is that it is, in principle, possible to apply it in two and three dimensions. There would probably be some differences, however. For example, unlike one dimension, the geometric mean of the equivalent to Eq. (12) for the two-dimensional square lattice is a function of energy which for a given ratio of t/V_0 may diverge for some energies and converge for others.[15] Thus, we expect a metallic and a insulating regime and an intermediate regime in which there exist mobility edges as predicted earlier.[15] Although, admittedly, the two- and three-dimensional cases require more study because the perturbation theory is more complicated, it appears quite likely that the nature of the metallic and insulating regimes will be qualitatively similar to that for the one-dimensional case. A more detailed discussion of the two- and three-dimensional cases will be presented in a future publication.

The physical reason for the localization for small t/V_0 can easily be understood. Because of the incommensurate nature of the system, an electron in a state of energy $V_0\cos Qn_0a$ at site n_0 will never be able to tunnel into a state of exactly the same energy and thus form extended bandlike states. For small V_0/t, V_0 becomes the perturbation on the extended bandlike states.

In actual practice it will be difficult to distinguish a high-order commensurate from an incom-

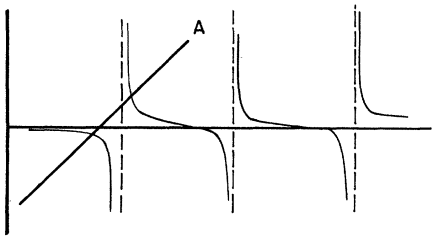


FIG. 3. A sketch is given of the right-hand side of Eq. (14) as a function of energy. The straight line labeled A represents a sample sketch of $E-V_0\cos(Qn_0+h)$.

mensurate system. For example, consider a high-order commensurate state for which sites degenerate with the site n_0 repeat every M sites. Divide the system into unit cells by bisecting the distances between these degenerate sites. Using Eq. (12) to calculate wave functions localized about sites n_0, $n_0'+M$, $n_0'+2M$, $n_0'+3M$, etc., at the boundaries between cells, we find that the overlap of wave functions localized in neighboring cells is $\sim(2t/V)^{2M}$. Thus, applying the tight-binding approximation to such a system we get bands of width $\sim(2t/V_0)^{2M}$. Between degenerate sites, however, the wave functions decay exponentially. Thus, if the system's size is smaller than one of the large unit cells (e.g., if the crystal is coherent over a distance smaller than Ma), it will be impossible to distinguish between incommensurate and high-order commensurate systems. That is, the bandlike states could still behave essentially as localized states over coherence regions smaller than Ma.

III. DISCUSSION OF EXPERIMENTAL CONSEQUENCES

The insulating state is characterized by exponentially localized wave functions, whose decay length becomes infinite as the transition is approached. Following the discussion in the book by Mott and Davis,[16] we would predict that at $T=0$, the dc electrical conductivity will be zero. As T increases, we find at low temperatures a conductivity proportional to $e^{-C/T^{1/2}}$, where C is proportional to $(V_0-2t)^{1/2}$ by applying the method of Mott and Davis to our localized states in one dimension. The ac conductivity will go approximately as ω^2 and the optical spectrum will be continuous. On the metallic side but close to the metal-insulator transition, there exist very narrow bands of extended states separated by gaps. As V_0 approaches $2t$, the bandwidth narrows, approaching 0 at $V_0=2t$. Thus, we would also expect the zero-temperature metallic conductivity to go to zero as V_0 approaches $2t$.

Because of the relatively narrow gaps near the metal-insulator transition, we would expect to observe Zener tunneling in the electrical conduction. We would also expect to observe in very pure materials the negative differential resistance and Stark or Bloch oscillations predicted by Esaki[17] for commensurate superlattice systems of long period because the Brillouin zones are also very narrow in the incommensurate system. To observe such oscillations requires that the frequency $eE/\hbar k_{\max}$, where e is the electric charge, E the electric field, and $k_{\max}$ the width of a Brillouin zone (which can be very narrow for incommensurate systems) be much larger than the reciprocal of the electron scattering time.

The one-dimensional model is applicable to the case of a three-dimensional crystal with a one-dimensional modulation, as shown in Ref. 15, provided we consider only electrical conduction in the direction of the wave vector Q of the modulation. In directions perpendicular to Q there will, of course, be no metal-insulator transition. Higher-dimensional cases will be considered in future publications.

The optical spectrum of the present model consists of interband transtions for $V_0<2t$. This will appear as a series of narrow peaks which grow in intensity and become closer together as V_0 approaches $2t$. This is substantiated by numerical calculations of the frequency-dependent conductivity using the continued-fraction method.[15] On the insulating side (i.e., $V_0>2t$), since the states are independent of wave vector (in the same way that the spectrum is independent of phase for $V_0<2t$), we expect to see a density-of-states-like broad spectrum. Most likely the metallic-state spectrum evolves smoothly into the insulating-state one.

What has been said here regarding electrons in incommensurate lattices is, in principle, applicable also to phonons in such systems.[14] In the phonon case, however, it is crucial to consider the rearrangement of the equilibrium positions of the ions in strong-coupling cases (the regime in which localization takes place). This will be the subject of future investigations.

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