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Localization in One-Dimensional Lattices in the Presence of Incommensurate Potentials

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The density of states and the localized or extended nature of the eigenstates is investigated in one-dimensional crystals with a modulation potential incommensurate with that of the underlying lattice. Studies of the transmission coefficient T and of the spatial dependence of the eigenstates show that even in one dimension it is possible to have a mobility edge. The implications of these results on experimentally measured quantities are also discussed.

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In recent years there have been many studies of crystals containing a modulating periodic potential of a period different from that of the underlying lattice.[1,2] Such modulations occur naturally in crystals containing charge-density waves or spin-density waves[2] as well as in ionic conductors[3] and finally it has become possible to grow crystals with such modulation by molecular-beam epitaxy[4] (superlattices). Such periodic modulations can be either commensurate or incommensurate with the underlying lattice. Both cases are of considerable interest theoretically and experimentally.

A crystal with an incommensurate modulation presents an interesting case, in that, strictly speaking, it does not possess translational order. In this respect it is like a disordered solid. However, unlike a disordered solid, it possesses lengths over which it almost repeats. Thus, an incommensurate crystal presents a case intermediate between an ordered and a disordered solid. It has been argued[5,7] that, within the one-dimensional (1D) one-band tight-binding model, with incommensurate modulation there exists a "metal-insulator" transition at a critical strength of the modulation, i.e., all the energy eigenfunctions are localized above the critical value, while all become extended just below it. Such behavior is unlike that of a disordered solid, for which all states are localized in 1D, or that of a commensurate crystal, for which all states are extended. Such a transition in the nature of the eigenfunctions—which may be induced experimentally in the same sample by, for example, external pressure—presents a very interesting theoretical possibility that is worth investigating.

It is the purpose of this Letter to examine the nature of the eigenstates of this model by studying the transmission coefficient T of the 1D system of size N. This technique is employed in the problem of electrical conductance of a 1D disordered crystal with very interesting results.[8-10] In the course of the present study, a detailed density-of-states (DOS) calculation was made, and the spatial dependence of the eigenstates was examined.

The model we consider is

$$\epsilon_n c_n + t(c_{n+1} + c_{n-1}) = E c_n , \tag{1}$$

where the energy at site n is $\epsilon_n = V_0 \cos(Qn)$, c_n

is the amplitude at site n, t is the hopping matrix element, V_0 is the modulation potential strength, Q is the wave vector of the modulation, and the lattice constant is taken to be 1. We also impose rigid boundary conditions to simplify the diagonalization of Eq. (1).

To decide the nature of the eigenstates of the model in Eq. (1), we first accurately calculated the DOS so the positions and widths of bands and gaps are known. With the DOS three independent tests were done to determine the nature of eigenstates.

(i) We study the transmission coefficient T of the system as the size of the system N increases for a given energy E, modulation strength V_0, and wave vector Q. For localized eigenstates $T \to 0$ as $N \to \infty$, while for extended ones $T \neq 0$ as $N \to \infty$. We want to mention that in this problem the study of the transmission coefficient T is considerably simpler than for the 1D random potential as we are dealing with a definite potential and thus all questions of ensemble averages[9,10] do not arise. On the other hand, because of some extremely narrow bands, special care is required in order to avoid calculating T at a gap and erroneously interpreting the result as showing the existence of localized eigenstates.

(ii) By directly diagonalizing[9] Eq. (1) for a given N, V_0, and Q, one gets the eigenvalue E and the corresponding eigenstate. In the present study, because of the one-dimensionality and the rigid boundary conditions, the matrix form of Eq. (1) is tridiagonal. Thus these eigenvalues and the corresponding eigenstates[9] can be easily calculated for systems up to 10 000. The accuracy of our eigenvalues and eigenstates is roughly sixteen and eight significant figures, respectively, with the double precision in the IBM machine. From the spatial behavior of the eigenstates, one can decide their nature, i.e., whether they are localized or extended. The application of this diagonalization method requires special care when there is almost degeneracy. We shall report elsewhere the related problems and the way we faced them.

(iii) One can approximate Q by $2nN/M$ (N,M integers without a common factor) so that after M sites the potential almost repeats. Consider the nth group of M consecutive sites (nth block). Within this group one can define $\epsilon_n^{(1)}$ as the eigenvalue closer to the energy under consideration and $t^{(1)}$ as the effective hopping-matrix element between wave functions of neighboring blocks. ($t^{(1)} = \langle \psi_n | H | \psi_{n+1} \rangle$, where $|\psi_n\rangle$ is the wave function of the nth block.) Since $|\psi_n\rangle = \sum_i c_{ni} |i\rangle$, where the ith summation is over the sites of the nth block, one obtains that $t^{(1)} = t c_{nM}^{\dagger} c_{(n+1)M}$. c_{nM} is the amplitude at the last site of the nth block, and $c_{(n+1)M}$ the amplitude at the first site of the $(n+1)$th block. In all the cases we examined $\epsilon_n^{(1)}$ is, within numerical uncertainties, of the form $V_0^{(1)} \cos(Q^{(1)} n + \varphi)$. This shows that under this transformation the original Hamiltonian matches to itself with transformed values of the parameters $V_0^{(1)}$ and $Q^{(1)}$. Our numerical results showed that for all values $V_0/2t > 1$, $V_0^{(1)}/2t^{(1)} > V_0/2t$, while for all values $V_0/2t < 1$, $V_0^{(1)}/2t^{(1)} < V_0/2t$ independent of the values of E and Q. Hence by repeating this transformation it follows that for $V_0 > 2t$ ($V_0 < 2t$) the Hamiltonian maps finally into $\lim_{n\to\infty} V_0^{(n)}/t^{(n)} \to \infty$ (0), which physically means that in the first case the states are localized and in the second case they are extended.

By combining for the first time the Green's-function technique for calculating the DOS, direct determination of eigenstates, and calculation of the transmission coefficient T, we avoided the common mistake of erroneously interpreting the gaps as localized states. It is indeed the consistency of the three complementary techniques which allowed us to decide with confidence about the nature of eigenstates.

For the case where $\epsilon_n = V_0 \cos(Qn)$ and Q is an irrational multiple of π our results show that $V_{0c}/t = 2$ is the critical modulation strength independently of E and Q in agreement with previous work.[5,6] For $V_0 > 2t$ all the states are localized while for $V_0 < 2t$ all the states are extended. In the localized regime one can define a decay localization length l_c either from the spatial decay rate of the eigenstate or from the length dependence of T as $L \to \infty$, which agrees with that proposed by Aubry,[6] i.e., $1/l_c = \ln(V_0/2t)$. It is surprising that V_{0c} is independent of E. From experience with random systems, one expects the states at the end of the band to become localized more easily than those at the center. On the other hand, for $\epsilon_n = V_0 \cos(Qn)$, the site energy spacing becomes smaller as we move towards the band edges and this facilitates propagation. It seems that, for the simple sinusoidal case, the two opposing tendencies cancel each other and the localization is independent of the energy. To check this physical explanation, we considered more complicated modulations, e.g.,

$$\epsilon_n = V_0[\cos(Qn) + V_1 \cos(2Qn)] \qquad (2)$$

with $V_0/t = 1.9$, $V_1 = \frac{1}{3}$, and $Q = 0.7$. The above

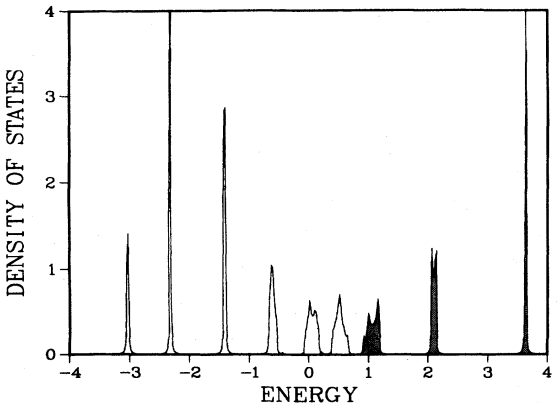

FIG. 1. The density of states (DOS) per site as a function of energy with $N = 20\,000$, $Q = 0.70$, $V_0 = 1.9t$, and $V_1 = \frac{1}{3}$. The shaded areas denote localized states.

argument suggests that, for ϵ_n given by Eq. (2), the eigenstates corresponding to high energies are easier to localize than those for low energies. By using the three methods which we described before we found that this is actually the case and that mobility edges exist. By using method (iii) we found that $\epsilon_n^{(1)}$ is given by $V_0^{(1)} = \cos(Q^{(1)}n + \varphi)$, but this time $V_0^{(1)}$ depends on energy E. For a given set of V_0, V_1, and Q (with V_0 less than a critical value) one has some of the eigenstates localized and some of them extended. In particular, as seen from Fig. 1, the states above $E = 0.70t$ are localized, while the rest are extended. Thus, our tentative conclusion is that the mobility edge lies in a gap. The form of the DOS cannot be used to differentiate subbands of localized states from those of extended states [see Figs. 2(a) and 2(c)]. On the other hand, the spatial behavior of corresponding eigenstates [see Figs. 2(b) and 2(d)] change drastically as we cross the mobility edges.

Following the argument of Ref. 5, one can obtain a rough approximate expression for the localization function $L(E)$, which becomes exact in the limit $L(E) \to 0$: $L(E) \simeq t/\langle \epsilon_n \rangle_g$, where

$$\langle \epsilon_n \rangle_g = \exp[(1/2\pi)\int_0^{2\pi} \ln|\epsilon(\varphi)|\, d\varphi],$$

and $\varphi = Qn$. Integrals of this type can be calculat-

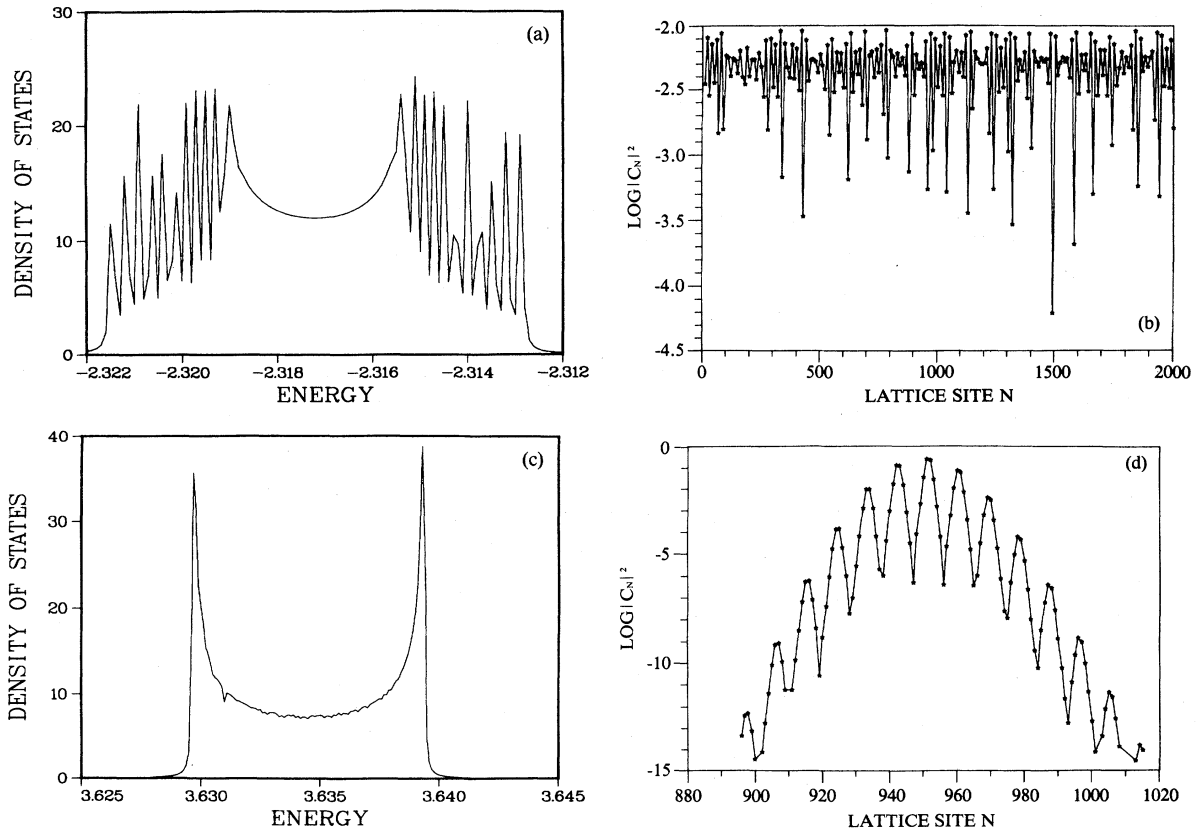

FIG. 2. (a), (c): Blowup of two subbands of Fig. 1. Typical (b) extended and (d) localized eigenstates corresponding to the centers of the subbands shown in (a) and (c), respectively.

ed by taking into account that, since $\epsilon(\varphi)$ is periodic and real,

$$\epsilon(\varphi)=\sum_{m=-N}^{N} G_m e^{im\varphi}=\sum_{m=-N}^{N} G_m Z^m \equiv \Pi_{2N}(Z)/Z^N,$$

where $Z=\exp(i\varphi)$, and $\Pi_{2N}(Z)$ is a polynomial of degree $2N$. If $Z_2, Z_4, Z_6, \ldots$ are the roots of $\Pi_{2N}(Z)$ which are outside the unit circle then

$$\tfrac{1}{2}\pi^{-1}\int_0^{2\pi} d\varphi \ln|\epsilon(\varphi)| = \ln|G_N Z_2 Z_4 Z_6 \ldots|.$$

Substituting, we have finally that $\langle \epsilon_n \rangle_g = |G_N Z_2 Z_4 \times Z_6 \ldots|$. For the simple case where $\epsilon(\varphi) = V_0 \cos\varphi$, we have $G_1 = V_0/2$, $|Z_2| = 1$, and hence $L(E) \simeq 2t/V_0$. In this case $L(E)$ happens to be exact. In more complicated cases, $L(E)$ can be reasonably estimated by rounding $t/\langle \epsilon_n \rangle_g$ over an energy range of the order of t (the rounding corrects for the omitted higher-order terms in t/V_0).

In conclusion, the main result of our work is that the presence of incommensurate modulations produces in general mobility edges in 1D systems. Thus experiments in (clean) thin wires with incommensurate modulations in which the Fermi level can be made to be either in extended regions or in localized regions, e.g., by applying pressure, offer the rare opportunity to study the role of localization (versus electron-electron correlations) in effects like the low-temperature excess resistance observed in disordered systems.[11]

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Influence of Spin-Orbit Coupling on Weak Localization

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The spin-orbit coupling modifies the weak localization of the conduction electrons in thin films and reverses the magnetoconductance. This is quantitatively demonstrated in Mg films covered with submonolayers of Au. The effect provides a new and direct method for measuring the spin-orbit coupling.

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After the pioneering work of Thouless[1] and Abrahams *et al.*[2] the localization of conduction electrons in $d \leq 2$ dimensions experienced a growing interest. In particular weak localization in two dimensions has been intensively studied theoretically[3] as well as experimentally.[4,5] In addition to the logarithmic divergence of the resistance at low temperature, the strong magnetoconductance which has been predicted by Altschuler *et al.*[6] and Hikami, Larkin, and Nagaoka[7] yields an excellent experimental possibility to study the weak localization. I expect that this state will become a most effective tool in the future to measure basic solid-state properties. The present paper describes a measurement of the spin-orbit coupling. In addition to the weak localization there is another low-temperature divergence of the resistance which is due to impurity-induced electron-electron interaction.[8] It can be distinguished from the weak localization by the magnetoconductance.[9]

A challenging problem in the theory of weak localization is presented by the spin-orbit coupling. Hikami, Larkin, and Nagaoka[7] calculated