Stark-Wannier resonances and delocalization in one-dimensional incommensurate systems with a finite electric field

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A model is explored for which weak electric fields are applied to crystals with incommensurate potentials in one dimension, within the localized regime. The results indicate a delocalizing effect due to the electric field, in agreement with tunneling models previously proposed for nonlinear conduction effects for the low-temperature semiconducting phase of quasi-one-dimensional solids and also yields a series of Stark-Wannier resonances found by other authors in different models. The effects of disorder tend to wipe out the resonances. The resonances would occur for somewhat higher values of electric field than the weak electric fields, sufficient to cause a delocalizing effect in the case of pure charge-density-wave crystals.

I. INTRODUCTION

It is known that crystals containing charge-density waves (CDW's), in their low-temperature, semiconducting phase, are characterized by a nonlinear conductance as a function of the applied field e. It is found that for $e \geq e_T$ where e_T is a threshold value, that the conductance may be described as[1,2]

$$G = G_a(e) + G_b(e - e_T)e^{-e_0/e} , \tag{1.1}$$

where G is the total conductance which eventually saturates to a value $G_a + G_b$ which would be observed in the absence of a CDW. The natural interpretation for the results for the conductance for weak fields obtained here is that it arises from a tunneling effect across the CDW-induced gaps, similar to the proposals of Bardeen.[3,4] One should remark, though, that other kinds of models have been proposed, such as CDW depinning,[5] so that the situation is still not clear.

We consider a one-dimensional tight-binding model for a CDW in which the localization length may be calculated. The calculation of G is carried out by postulating that the Landauer formula is still valid for strongly localized states with weak applied fields for which the tunneling effect is indeed found. For slightly larger values of electric field a series of Stark-Wannier resonances are found in $\gamma(e)$ (the inverse localization length as a function of the applied field) and are similar to the Stark resonances found by other authors in different models. In particular much work has been done on a nearly-free-electron model containing a distribution of delta functions.[6,7]

It has been pointed out that translational invariance is not prerequisite in finding Stark resonances, since these are observed also in disordered models.[8] It comes as no surprise then that they turn up also in incommensurate CDW structures. Nonlinear effects are also found in the conductance of superlattices[9] and this model may also be applicable there.

II. THE MODEL

We consider a linear chain with nearest-neighbor hopping matrix element V. The diagonal site energies are taken according to

$$\varepsilon_n = \varepsilon_n^0 - nea e , \tag{2.1}$$

where

$$\varepsilon_n^0 = W \cos(Qna) \tag{2.2a}$$

or

$$\varepsilon_n^0 = W \,\mathrm{sgn}[\cos(Qna)] , \tag{2.2b}$$

where sgn is the sign(um) function, $Q = 2\pi/\lambda$, where λ is the period of the CDW, and W is the amplitude of the CDW. Off-diagonal corrections due to the electric field can be neglected only for weak electric fields.

There is also an important factor to be considered when calculations are performed with a finite electric field. This is the fact that as a result of band tilting the electron is confined within a distance $l_B = B/ee$ due to Bragg reflection at band edges. (This is in the absence of phonons.) One can state then that two regimes are of interest depending on the electric field e and localization length l.

(i) Material effects dominate when $l < l_B$.

(ii) The electric field dominates when $l_B < l$.

In this work we limit the study to region I, which translates into the condition $eea/B < \gamma$ where B is the total bandwidth, γ the inverse localization length, and a is the lattice spacing. Region II is probably physically unrealistic in the absence of phonons which would help the electrons to conduct in the presence of the field.

With diagonal site energies $(\varepsilon_1, \varepsilon_2, \varepsilon_3, \ldots)$ a continued-fraction expansion for the right self-energy is given by

$$\Delta_0^+ = \cfrac{V^2}{E-\varepsilon_1-\cfrac{V^2}{E-\varepsilon_2-\cfrac{V^2}{E-\varepsilon_3-\cfrac{V^2}{\cdots}}}} . \tag{2.3}$$

The CDW is taken to be incommensurate with $\lambda=\pi a$ giving $\varepsilon_n^0=W\cos(2n)$ or $\varepsilon_n^0=W\,\mathrm{sgn}[\cos(2n)]$ potential. In the case of $W\cos(Qna)$ it is well known that there is a metal-insulator transition for $e=0$ at $|W|=2V$.[10,11] Since the calculations must be carried out in the localized regimes one takes $|W|>W_c=2V$. The effects that we find can only be qualitatively correct since W_c is about 50 times larger than the actual observed order parameter for the metal-insulator transition. The discrepancy is probably due to shape distortions from the cosine and three-dimensional effects. Thus for the rectangular potential states with very small W are already localized.

The localization length can be taken as the convergence length of (2.3),[12,13] for which the difference between successive convergents is less than a given error ϵ:

$$\left|\frac{1}{Q_nQ_{n+1}}\right| = \left|\frac{P_{n+1}}{Q_{n+1}}-\frac{P_n}{Q_n}\right| < \epsilon .$$

Simple recursion relations can be given for P_n and Q_n:

$$\begin{aligned} P_{n+1}&=a_{n+1}P_n+P_{n-1} , \\ Q_{n+1}&=a_{n+1}Q_n+Q_{n-1} . \end{aligned} \tag{2.4}$$

For the special case of exponential localization (strongly localized states) one can assume the following divergence for P_n and Q_n as a function of n:

$$P_n^2+Q_n^2 \propto e^{\gamma n} .$$

Although γ is perfectly well defined in the absence of an electric field this is no longer necessarily so when $e\neq 0$. It seems safer then to use the criteria that l is attained when $P_n^2+Q_n^2$ is larger than some predetermined large number. In (2.4) a_n is given by

$$a_n=(-1)^n\left[\frac{E-\varepsilon_n}{V}\right] . \tag{2.5}$$

In practice it was found that for strongly localized states there was exponential localization which remains so for weak electric fields, although a change to a power-law localization is expected for larger fields.

Calculation of γ must, however, be limited to a sufficiently short length to avoid the region in which the e field is dominant. The limit on electric field depends on the localizing potential. In the case of the cosine one has $eaeL/B<\ln(W/W_c)=\gamma$. For short lengths and $e\neq 0$, γ does not depend on the length that is used. However, since sufficiently long lengths always cause the electric field effect to dominate it is necessary to limit this length.

Due to band tilting of the finite band the states will appear to be localized even in the normally extended region $W<W_c$, so as mentioned previously an obvious requirement to see material dominated effects is $L<l_B$ where L is the sample length. It is also apparent that as long as the variation of electrical potential eeL is negligible compared to fluctuations of the effectively localizing potential, that states should still be exponentially localized within L. Numerically one checks the exponential convergence of the continued fraction. Thus while the transition to power-law localization is never really seen in this model, due to the single initial band, the physical requirement to see exponentially localized states remain $eaeL/B<\gamma$ and $L<l_B$.

III. RESULTS

We summarize our results as follows.

(a) Results without an electric field are given in Figs. 1(a) and 1(b) in the case of Eqs. (2.2a) and (2.2b), respectively. The results are in agreement with previous calculations.

(b) There is a delocalization for weak electric fields given by $\gamma(e)=\gamma(0)-Ae^{-e_0/e}$ where $A>0$ is a constant which occurs in the region of strongly localized states (Fig. 2). The fit is made allowing only a very small per-

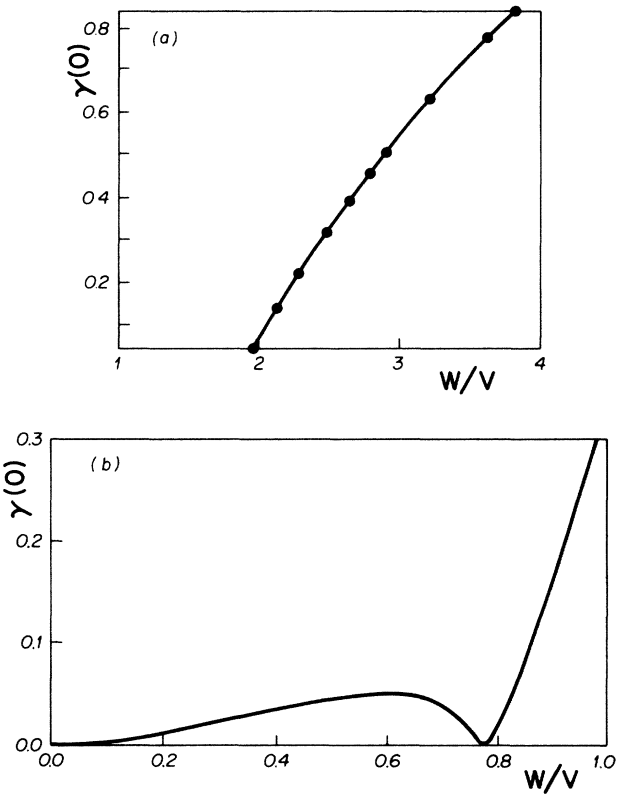

FIG. 1. (a) This figure shows the inverse localization length γ as a function of W/V for $e=0$ for the potential $\varepsilon_n=W\cos(2n)$. The metal-insulator transition is not exactly at $W_c/V=2$ only because of the finite length used in the numerical calculations. $\gamma=0$ for $W<W_c$. The theoretical expression for $W>W_c$ is $\gamma=\ln(W/W_c)$. (b) This figure shows $\gamma(e=0)$ as a function of (W/V) for the potential $\varepsilon_n=W\,\mathrm{sgn}[\cos(2n)]$. States very close to $W=0$ are now localized. The overall behavior is intermediate between that of an uncorrelated rectangular distribution for the ε_n's and that of a cosine.

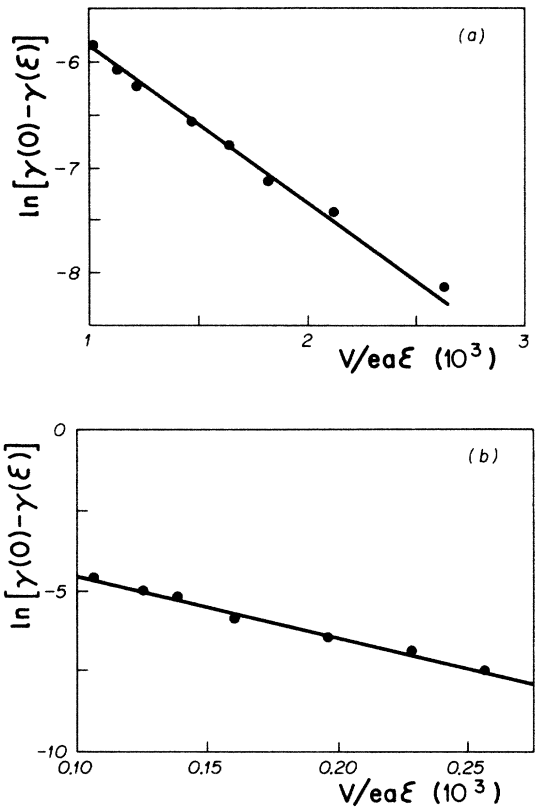

FIG. 2. (a) This figure shows $\ln[\gamma(0)-\gamma(e)]$ plotted as a function of V/eea for $W/V=1.2$ with $\varepsilon_n^0=W\,\mathrm{sgn}[\cos(2n)]$. A length of up to $100a$ was used to perform the calculations and $\gamma(e)$ was obtained by assuming exponential localization. A linear fit giving $eae_0/V=1.49\times10^{-3}$ is obtained. (b) This also shows $\ln[\gamma(0)-\gamma(e)]$ vs V/eea but for $W/V=2.0$ with $\varepsilon_n^0=W\,\mathrm{sgn}[\cos(2n)]$. Lengths of up to $100a$ were used to find $\gamma(e)$ which was obtained assuming exponential localization. The fit is linear giving $eae_0/V=2.07\times10^{-2}$. The tendency is for e_0 to increase with degree of localization.

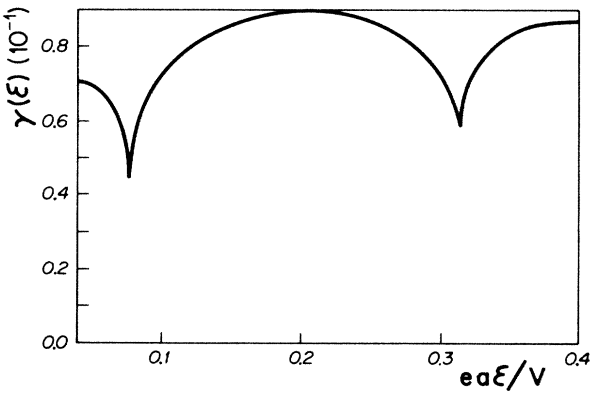

FIG. 3. This is a typical run showing $\gamma(e)$ as a function of (eae/V). Here the continued fraction was evaluated until the difference between successive convergents was less than 10^{-6}. The calculation was carried out with $W/V=3.0$ and $\varepsilon_n^0=W\cos(2n)$. Stark-Wannier resonances are present.

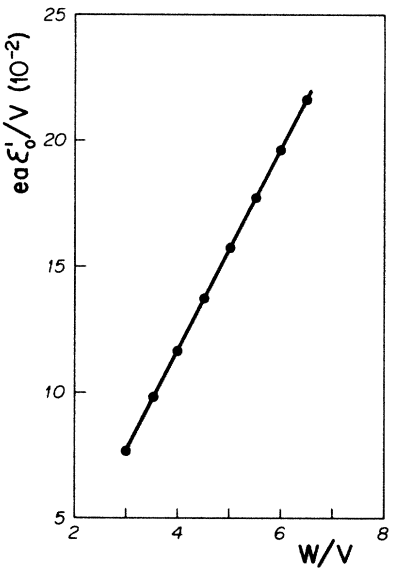

FIG. 4. This figure shows the position of a Stark-Wannier resonance eae_0'/V as a function of W/V for $\varepsilon_n^0=W\cos(2n)$. The resonance moves linearly to the right as a function of the CDW amplitude. The behavior of e_0' for smaller values of W/V than those shown are not clearly interpretable.

centual change in $\gamma(0)$ due to e.

(c) A series of Stark-Wannier resonances occur for larger fields (see Fig. 3). The position of the first such resonance is named e_0'.

(d) Both e_0' and e_0 increase with the degree of localization. The increase of e_0' is linear in W for the case of $\varepsilon_n^0=W\cos(Qna)$. (See Fig. 4.)

(e) The Stark-Wannier resonances tend to disappear when disorder is added: $\varepsilon_n^0=W\cos(Qna)+W'$ where W' has a rectangular distribution.

(f) Strongly electric fields cause γ to rise again due to the band tilting effect (region II).

(g) Another interesting result is that the approximate $L(E)$ method works surprisingly well. It is of course known to be exact with $\varepsilon_n^0=W\cos(Qna)$ and no electric

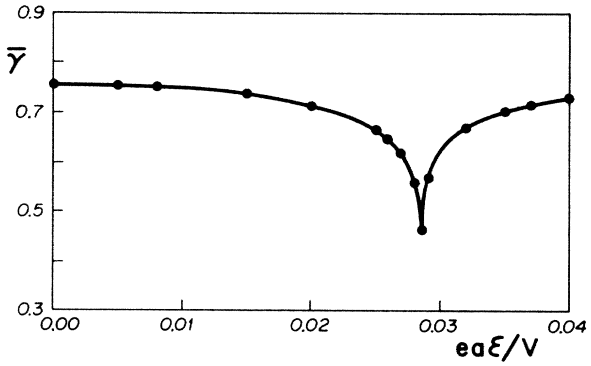

FIG. 5. This figure shows γ' found by applying the $L(E)$ method for $W/V=4$ as a function of eae/V calculated from lengths up to $25a$. Delocalizing behavior and resonances are seen.

field. Indeed if we consider

$$H(J)=\ln\left[\prod_{n=1}^{J}\left|\frac{E-W\cos(2n)-ea\,en}{V}\right|\right]$$

with $E=0$ and $e=0$, $H(J)$ is an increasing function of J for $W>2V$ but decreases with J for $W<2V$. In Fig. 5 we have found γ' from fitting $H(J)=\gamma' J$ for $E=0$ and $W/V=4$ for values of J up to 25. The behavior of γ' as a function of e again shows the delocalizing effect for small e and Stark-Wannier resonances. The delocalizing field is also seen in that the value of the critical amplitude (W_c/V) increases from its value of 2, as the electric field is increased.

IV. INTERPRETATION AND DISCUSSION

For large values of W it can be thought that each dip in the CDW potential contains independent energy levels. The band-tilting effect due to the electric field lines up some of these levels leading to the resonances. Evidently the separation of these levels is larger when W is larger, leading to a higher value of ε_0'. For strongly localized states one can approximate G by $G\simeq e^{-\gamma L}$ where L is the sample length.

Substituting $\gamma(e)=\gamma(0)+[\gamma(e)-\gamma(0)]$ and considering weak fields only

$$\begin{aligned}G&\simeq e^{-\gamma(0)L}e^{-L[\gamma(e)-\gamma(0)]}\\&\simeq e^{-\gamma(0)L}\{1-L[\gamma(e)-\gamma(0)]\}\\&\simeq e^{-\gamma(0)L}(1+LAe^{-e_0/e})\,.\end{aligned}$$

This leads naturally to the separation of G into a G_a and $G_b e^{-e_0/e}$.

Despite the apparent success of the model in giving a Zenner-like contribution due to tunneling between minibands (spectrum split up by the CDW) in which the tunneling distance goes as $1/e$, the assumption that the Landauer formula can be used for $e\neq 0$ is not proven. Further theoretical work is needed in the field to establish this. Another problem is to find precise ways of defining γ when $e\neq 0$. If calculated as it usually is, γ is still found to be somewhat dependent on position; the wave function would go as $\psi\sim e^{-\gamma(x)x}$ to which one must add the complication of the changing character of the localization as a function of e.

On the basis of our results we would say that γ is still fairly well defined, at least for weak fields and strong localization, and that in this limit the Landauer calculation of G seems reasonable. One could say that weak fields do not alter the exponential character of the delocalization and therefore linear response (on the basis of which the Landauer formalism stands) is still valid about a new situation in which there is a small applied field.

One notes that the threshold field itself e_T is expected to arise from impurities so it is essentially zero ($e_T=0$) in the pure case. It should also be noted that the fit $\gamma(e)=\gamma(0)-Ae^{-e_0/e}$ is only good for strongly localized states but not for nearly extended states. In this latter case there is complicated behavior which is not easily analyzed since the modulated part of $\gamma(x)$ becomes important.

It suffices to note that when the electric field is dominant (region II), this scheme breaks down. Actually this is a difficult regime for nearly free electrons also. Despite the fact that in this later case the effect of finite potentials will always be felt, even for very large sample lengths, the electron always acts as if it were nearly free if it moves a large enough distance. Then what is missing in this later model are phonons to help slow these down while in our model phonons would be needed to help electrons to move along.

The results which were obtained are quite different from those of Refs. 7 and 8, but the model we use is also very different. References 7 and 8 use a model more appropriate to nearly free electrons and their states are more extended (power-law localized in the presence of impurities). The present model is a tight-binding formalism where exponential localization is obtained in the strong-potential limit ($W>2V$ for the cosine) or when impurities are added. Our single band is completely split up into minibands by the CDW while the other models have an essentially semi-infinite band structure.

With exponentially localized states the local order has a much stronger effect on the results so that it is not surprising that the resonances disappear with disorder (while they persist in the other models). Alternatively, if the energy levels of the successive wells are regarded as approximately independent, addition of disorder means that they are resonant only two at a time, instead of all being resonant (constant energy shifts from one level to the adjacent one) due to the e-field tilting effect.

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