Tuning of dynamic localization in coupled mini-bands: signatures of a field induced insulator-metal transition

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We follow the evolution of dressed coupled mini-bands as a function of an AC field intensity, non perturbatively, for a wide field frequency range. High and low frequency limits are characterized by two different dynamic localization regimes, clearly separated by a breakdown region in a quasi-energy map. Signatures of an insulator-metal like transition by means of a field induced suppression of a Peierls-like instability are identified.

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The behaviour of semiconductor micro-structures driven by intense AC fields, has been of renewed interest, from both theoretical and experimental points of view, in the past few years. This subject, originally addressed in the context of atomic and molecular physics, raised the question of how these effects would appear in a periodic lattice, where the atomic levels are broadened into bands. Among the theoretical predictions, we pay special attention on a pioneering one\textsuperscript{1}–\textsuperscript{5} which consists in the transformation of isolated bands, leading to dynamic localization in finite superlattices (SLs). The period of these SLs are typically orders of magnitude shorter than the radiation wavelengths for energy scales mentioned above. Consequently, the dipole approximation holds and suggests a common framework for superlattices driven by intense FIR lasers or by high frequency bias.

The problem of multi-mini-bands has also been initially addressed few years ago by Holthaus and Hone\textsuperscript{1}. The same authors suggest an interesting possibility in the context of atomic and molecular physics: at zero field and for low frequency field, the dimerization is suppressed and an analog to an insulator-metal transition takes place.

We focus on a heuristic two-mini-band model in the presence of a strong AC electric field, within a tight-binding framework, emulating the dimerized SL proposal\textsuperscript{1}. A linear chain is considered for this SL, where each single “atomic” s-like orbital of the site is associated to one quantized level energy of a QW. The hopping parameters describe the coupling between the QW levels through the SL barriers. The applied AC fields are parallel to the chain. Hence, our model is described by the Hamiltonian $H = H_0 + H_{\text{int}}$, considering nearest neighbour interaction only:

$$H_0 = \sum_\ell \epsilon_\ell |\ell><\ell| + \frac{V}{2} \sum_\ell \left[ |\ell><\ell+1| + |\ell+1><\ell| \right]$$

$$H_{\text{int}} = e a F \cos \omega t \sum_\ell |\ell > \ell < \ell|$$

where $\epsilon_\ell = (-1)^\ell E_g/2$, $E_g$ is the mini-band gap energy at zero field and $\ell$ is the index site; $\omega, F$ are the AC field frequency and amplitude, respectively. $a$ is the SL period, $e$ is the electron charge. For $E_g = 0$ one has the single band limit, while for $E_g \neq 0$ one has a dimerized SL with a $2\pi$ period. The treatment of the time-dependent problem is based on Floquet states $|\ell, m\rangle$ where $m$ is the photon index. We follow the procedure first developed by Shirley\textsuperscript{1}, which consists in the transformation of the time-dependent Hamiltonian into a time-independent infinite matrix which must be truncated. The matrix elements are:
\[ [(\mathcal{E} - m\hbar\omega - \epsilon_{\ell})\delta_{\ell,\ell'} - \frac{V}{2}(\delta_{\ell,\ell-1} + \delta_{\ell,\ell+1})]\delta_{m',m} = \\
F'\delta_{\ell,\ell'}(\delta_{m',m-1} + \delta_{m',m+1}) \quad (3) \]

where \( F' = \frac{1}{2}eaF \). The dimension of the matrix is \( L(2M + 1) \), where \( L \) is the number of atomic sites, while \( M \) is the maximum photon index. We choose \( M \) in order to satisfy a convergence condition: symmetric spectra relative to the Quasi Brillouin Zones (QBZs) edges. The first QBZ is spanned in the range \(-\hbar\omega/2 \leq \mathcal{E} \leq \hbar\omega/2\).

In what follows we show, initially, quasi-energy spectra as a function of the electric field intensity. It is important to notice that in this work we choose to keep the field frequency constant \((\hbar\omega = 0.5 \text{ meV})\), corresponding to \( \nu \approx 0.1 \text{ THz} \), while “tuning” the SL (varying \( E_g \), with \( V = 0.2 \text{ meV} \) fixed). This reveals, as will be seen, to be a useful procedure for a clear identification of different dynamic localization signatures, for the whole range from \( E_g/\hbar\omega \ll 1 \) to \( E_g/\hbar\omega > 1 \).

In Fig.1, examples of quasi-energy spectra as function of field intensity are shown. In all cases the chains are \( L = 20 \) sites long. Fig.1(a) presents the limit of \( E_g = 0 \), i.e., a single and isolated mini-band. The collapses coincide with zeros of the Bessel function, \( J_0(eaF/\hbar\omega) \), \( (eaF/\hbar\omega: 1.2/0.5 = 2.4, 2.75/0.5 = 5.5, 4.32/0.5 = 8.64, \text{ etc.}) \) reproducing a single mini-band analytical result: \( \mathcal{E}(k, \omega) = 2VJ_0(eaF/\hbar\omega)\cos ka. \) This result follows the replacement \( \hbar k \rightarrow \hbar k - eA(t) \). Fig.1.(b) shows the spectra of two mini-bands formed by the dimerization procedure with \( E_g = 0.10 \text{ meV} \), i.e., the limit \( E_g/\hbar\omega \ll 1 \), even conserving remnants of the collapses at zeros of \( J_0(eaF/\hbar\omega) \), analytically described, considering the same momentum substitution above by:

\[ \mathcal{E}(k, \omega) = \pm 2[(E_g)^2 + V^2J_0^2(eaF/\hbar\omega)\cos^2 (ka/2)]^{1/2}. \quad (4) \]

But, a dimerized SL with \( E_g/\hbar\omega \sim 1 \) shows a qualitative different behaviour: first, each mini-band collapses at values of \( F \) near to corresponding first zero of \( J_0(e2aF/\hbar\omega) \), since now the SL period doubles, this first collapse should occur at \( eaF \approx 0.6 \text{ meV} \), and this is already noticeable for \( E_g \approx \hbar\omega \). In all cases, \( V = 0.2 \text{ meV} \) and \( E_g = 3 \text{ meV} \), respectively. Atomic energies are varied, in order to increase the mini-band-gap \( E_g \) from top to bottom: (a) \( E_g = 0 \) (single band limit); (b) \( E_g/\hbar\omega = 0.1 \text{ meV}/0.5 \text{ meV} = 0.2 \); (c) \( E_g/\hbar\omega = 0.5 \text{ meV}/0.5 \text{ meV} = 1.0 \); and (d) \( E_g/\hbar\omega = 1.5 \text{ meV}/0.5 \text{ meV} = 3.0 \).

Some light may be shed on the problem by comparing mini-band spectra to the spectra of the corresponding single dimer unit of the SL. In Fig 2(a), the mini-band spectra of Fig.1(d), \( E_g/\hbar\omega = 3 \), (small dots), are compared to the spectra of the two level system corresponding to one dimer (large dots) that constitutes the SL. In Fig 2(b) the same is shown for \( E_g/\hbar\omega = 3.2 \) (out of three-photon resonances). Having in mind the dimer spectra, we see that replicas of these levels cross or anti-cross at the same intensities as the mini-bands anti-cross. Perfect crossing occur only for the two level system when \( E_g/\hbar\omega = n \), according to the von Neumann-Wigner rule. Observing the SL and isolated dimer spectra, after the breakdown of the mini-bands \( (eaF \approx 1.5 \text{ meV}) \),

![FIG. 1. Quasi-energy spectra as a function of field intensity for different chains L = 20 sites long. Hopping parameters and field frequency are the same in all cases, V = 0.2 meV and hω = 0.5 meV, respectively. Atomic energies are varied, in order to increase the mini-band-gap E_g from top to bottom: (a) E_g = 0 (single band limit); (b) E_g/\hbar\omega = 0.1 meV/0.5 meV = 0.2; (c) E_g/\hbar\omega = 0.5 meV/0.5 meV = 1.0; and (d) E_g/\hbar\omega = 1.5 meV/0.5 meV = 3.0.](image-url)
a new dynamic localization mechanism shows up due to the dominant behaviour of the dimers that constitute the SL and not to a field effect on the bulk as implicit in analytical results, like Eq.1. It is interesting to notice that this dominant dimer effect signature alternates with field induced mini-band gap collapses. Both effects occur only for $E_g/h\omega = n$ ($n$-photon resonances). Indeed, the crossing of the dimer level replicas occur at zeroes of $J_n(eaF/h\omega)$. The apparent crossings of the mini-bands at the QBBZ edges are actually anti-crossings not resolved in the figure. Detuning the $E_g/h\omega = n$ condition, Fig.2(b), the mini-band gap collapses disappear and the dynamic localization due to the dominant behaviour of the dimers evolves in a double collapse structure. This last result, Fig.2(b), was previously observed in Fig.6 of reference[4] where the authors take into account the SL potential profile explicitly. Resuming, these results lead to the following picture: the two mini-bands behave as isolated ones, only in the limit $E_g/h\omega > 1$ and below the mini-band electric breakdown range. At higher field intensities dynamical localization manifests as a decoupling of the SL in the constituting dimers, leading to multi-photon resonances between dynamically localized states. A related effect are the mini-band gap collapses at certain field intensities, for which the mini-band dispersions are maxima, when $E_g/h\omega = n$.

Near $E_g = 0$ we see the dark spots at $eaF$ values corresponding to the single band collapse of Fig.1(a). For $E_g > 1$ meV collapsing of individual mini-bands of the dimerized SL appear at zeroes of $J_0(eaF/h\omega)$, indicated by grey vertical lines. These collapses appear successively with increasing $E_g$ in the range $E_g > eaF$. Indeed, slightly below the $E_g = eaF$ diagonal a bright region indicates the dynamic breakdown regime, separating collapses of qualitative different evolution in the quasi energy spacing map. For $E_g < eaF$ the positions of mini-band collapses are functions of the field intensity: these are collapses related to the dominant behaviour of the dimers. The single spots at $E_g/h\omega = n$ are for crossings in the two level (dimer) systems. The two dark lines connecting single spots are the double collapsing structure that evolves out of the resonance condition, like in Fig.2(b). The horizontal grey lines at the left reflect an approximately constant degeneracy of surface states, for field intensities up to the dynamical breakdown, when mini-band replica strongly overlap in this representation. In this map, the upper left and lower right half-planes represent qualitatively different physical situations; respectively the isolated mini-band regime and a regime of field induced rearrangement of the electronic structure.

![FIG. 2. Quasi-energies as a function of field intensity, comparing finite chains (small dots), $L = 20$ sites long, with corresponding dimers, two level systems (large dots). (a) $E_g/h\omega = 1.5$ meV/0.5 meV = 3.0; and (b) $E_g/h\omega = 1.6$ meV/0.5 meV = 3.2.](image1)

This picture for the evolution of dressed mini-bands, is clearly illustrated by analyzing the projection of mini-band width $\Delta$, mapped on a $E_g$ versus $eaF$ plane shown in Fig.3, with $h\omega = 0.5$ meV fixed, while we are "tuning" the SL mini-band gap, considering a fine mesh for varying $E_g$. In the brightness scale, dark is for very small mini-band width, indicating mini-band collapses, and white is for large mini-band width, i.e., field intensity versus $E_g$ regions of relative maximum mini-band broadening.

![FIG. 3. Projection of the mini-band width $\Delta$ on a $E_g$ versus $eaF$ representation plane. The brightness scale spans from black (small $\Delta$: collapsing mini-bands) to white (widest $\Delta$: large mini-band dispersion).](image2)

This mapping refers to the mini-band dispersion, indicating clearly the evolution of mini-band collapses from one dynamic localization regime into another as a function of field intensity. However, there are also important mini-band gap variations, which apparently approaches zero in the main breakdown region, as well as in the "satellite" breakdown regions, when $E_g/h\omega = n$, as can be seen in the case of Fig.2(a). Referring to Fig.2(a),
one sees that at the intensities for which the mini-band gaps seem to collapse, the spectra resembles a single band density of states. For this reason, quasi-energy spectra as densities of states for selected field intensities for the case shown in Fig.2(a) are depicted in Fig.4. We clearly see a transition from a two mini-band density of states, Fig.4(a), (low field intensity range) to a single band density of states, Fig.4(c). Increasing further the field intensity, the two mini-band situation can be recovered, Fig.4(d). The shape of the density of states, shows an effective electronic structure alternating from binary (Peierls instability) to single (suppression of Peierls instability) band with field intensity. Such effect is an AC field tunable Peierls instability. This opens the possibility of a new insulator-metal transition, considering dimerized SLs doped in such a way that the first bare mini-band is fully occupied. Since it has been shown that consequences of band collapses in a single-band tight-binding model survives in the presence of Coulomb interactions, one could expect to observe insulator-metal like transitions in such dimerized SLs driven by tunable intense fields in the THz range.

FIG. 4. Density of states obtained from quasi-energy spectra at given field intensities, using a Breit-Wigner fit, for the case depicted in Fig.1(d). (a) $eaF = 0.3$ meV, (b) $eaF = 1.5$ meV, (c) $eaF = 2.2$ meV, and (d) $eaF = 2.55$ meV.

Other results, based on a different heuristic model, do not show a clear dynamic breakdown and signatures of isolated mini-bands behaviour survive up to very intense fields. These results consider also alternation in barrier thicknesses and, therefore, do not necessarily contradict the present ones. Including alternation of hopping parameters to our model, a similar picture to these previously reported results is obtained. The comparison of the present results with some previous reported ones suggests that further work is still necessary in order to build up a systematic understanding of the behaviour of dressed coupled mini-bands.

In summary, we showed the existence of two dynamic localization regimes in SLs dimerized by alternating well widths. No memory of the low field regime survives beyond the dynamic breakdown region, where a insulator-metal transition may occur as a consequence of the suppression of a Peierls-like instability for resonance field frequencies.

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