Avoided Band Crossings:
Tuning Metal-Insulator Transitions in Chaotic Systems

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We show that avoided crossings of energy bands may give rise to a variety of phenomena such as transitions from metal to insulator and vice versa, changes in localization lengths, and changes in the fractal dimension of energy spectra. We explain the occurrence of these phenomena in the kicked Harper model under classically chaotic conditions and predict them to occur in other systems.

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Spatially periodic quantum systems give rise to energy bands and extended eigenfunctions, according to Bloch’s theorem. If this periodicity is broken by a weak perturbation, e.g., by disorder or a (magnetic) superlattice, the spectrum remains band-like. Typically, one neglects the coupling of these "bands" and studies them in a one-band approximation. Prominent examples from solid state physics for such one-band models are the Anderson model for disordered systems\textsuperscript{1} and the Harper model for Bloch electrons in a magnetic field\textsuperscript{2}, which display such interesting properties as localized eigenfunctions or metal-insulator transitions. As a function of an external parameter some of these "bands" will move up in energy whereas others move down, thus giving rise to band crossings. At these crossings the coupling of bands can no longer be neglected and will lead to avoided band crossings (ABCs) in analogy to the well-studied avoided level crossings. The question then arises: Will these couplings of bands and in particular the ABCs change the properties derived in the simplifying one-band models?

A seemingly unrelated problem has occurred in the quantum chaos literature, while studying the influence of classical chaos on quasiperiodic quantum systems. Specifically, in the kicked Harper model (KHM)\textsuperscript{3,4}, it was found numerically that in the regime, where the classical limit is chaotic, extended eigenfunctions show up for parameters where exclusively localized ones were expected and vice versa\textsuperscript{5,6}. In addition, chaos was found to change the fractal dimension of the spectrum\textsuperscript{3,4}. In the absence of an explanation these puzzling phenomena have remained mysterious, and one may wonder: How can classical chaos induce such drastic changes in these quantum properties?

In fact, it will turn out here that the main impact of classical chaos is to generate ABCs and thus this question for the quantum chaos problem will be reduced to the previous question posed for the solid state problems. In the main part of this paper we therefore analyze avoided crossings of \textit{one-band models}. Although simple generalizations of avoided level crossings, these ABCs unexpectedly generate transitions from localized to extended eigenfunctions and vice versa and changes in the localization lengths of eigenfunctions as well as in the fractal dimensions of spectra. We show that ABCs cause these phenomena by effectively changing the parameters of the one-band models involved. We will demonstrate that these general findings can be applied to the KHM and thereby give the first explanation for the phenomena that were observed numerically in this model. Application to the old problem of Bloch electrons in a magnetic field\textsuperscript{2} leads to the prediction of dramatic effects, e.g., a wave packet spreading in one direction will, due to ABCs, spread in the perpendicular direction. These effects give rise to experimental consequences for transport measurements in semiconductor nanostructures and will be described in detail elsewhere\textsuperscript{16}. In the future we expect applications to coupled one-dimensional chains and many other systems.

Let us start by studying an ABC when there is no perturbation and the system is still periodic. Then each

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{An ABC with twist modeled by the Hamiltonian (\textsuperscript{8}), with $E' = -\cos k$, $E'' = \cos k$, and $\epsilon = 0.6$. The eigenvalues form two energy \textit{bands} for the set of all Bloch phases $k$. Arrows indicate in which direction the energies change as $k$ is varied from 0 to $\pi$. Solid and dashed lines represent the eigenvalues for $k = 0$ and $k = \pi$, resp. The inset shows an ABC without twist for the case $E' = E'' = -\cos k$ with $\epsilon = 1.4$.}
\end{figure}
band is described by a dispersion $E(k)$ depending on the Bloch phase $k \in [-\pi, \pi]$. Now, an isolated avoided crossing of two bands can be modeled by the Hamiltonian

$$H = \begin{pmatrix} E^+(k) + A - \lambda & \epsilon & 0 \\ \epsilon & E^0(k) + \lambda & \epsilon \\ 0 & \epsilon & E^-(k) - A - \lambda \end{pmatrix},$$

(1)

where $\epsilon$ is the coupling parameter. For any fixed Bloch phase $k$, $H$ simply models an avoided level crossing. When looking at the entire band there are two cases of interest: If the dispersion relations of the two bands have the same general dependence on $k$, namely $\frac{dE^+}{dk} > 0$ for $k \in [0, \pi]$, the resulting spectrum resembles that of a broadened avoided level crossing (see inset of Fig. 1). In the alternative case of opposite general dependencies on $k$, namely $\frac{dE^+}{dk} > 0$ and $\frac{dE^-}{dk} < 0$ for $k \in [0, \pi]$, each band is twisted (Fig. 1).

Two subsequent ABCs with twist (see Fig. 2a) can be modeled by the Hamiltonian

$$H = \begin{pmatrix} E^+(k) + A - \lambda & \epsilon & 0 \\ \epsilon & E^0(k) + \lambda & \epsilon \\ 0 & \epsilon & E^-(k) - A - \lambda \end{pmatrix},$$

(2)

where a rising band $E^0$ subsequently crosses two decreasing bands $E^-$ and $E^+$ with offsets $\pm A$. For small coupling $\epsilon$ the two twists of the intermediate band are well separated, whereas for increasing $\epsilon$ they first come closer whereby the band flattens, which will be important later on, and finally the twists annihilate (Fig. 2).

We now show the dramatic effect of ABCs in the presence of a weak perturbation. This we model by the Hamiltonian of Eq. (2) with the bands $E^{\pm,0}(k)$ replaced by Hamiltonians $H^{\pm,0}$, leading to the Hamiltonian

$$H = \begin{pmatrix} H^+ + A - \lambda & \epsilon & 0 \\ \epsilon & H^0 + \lambda & \epsilon \\ 0 & \epsilon & H^- - A - \lambda \end{pmatrix}.$$

(3)

For simplicity, we will focus on tight-binding Hamiltonians $H^{\pm,0} = \sum_n V^\pm_n a_n^\dagger a_n + \sum_n t^{\pm,0} \left( a_{n+1}^\dagger a_n + a_{n-1}^\dagger a_n \right)$ on one-dimensional lattices with spatially varying on-site potential $V^\pm_n$ and with hopping terms $t^{\pm,0}$. For zero on-site potentials ($V^\pm_n \equiv 0$) Eq. (3) reduces to Eq. (2) studied in Fig. 2.

As a first numerical example we assume $H^0$ according to Harper’s model for Bloch electrons in a magnetic field $\mathbf{B}$ in the metallic regime, i.e., we take the on-site potential $V^0_n = V^0 \cos(2\pi \sigma n)$ and $V^0 \equiv 0 < 2$, where $\sigma$ is the magnetic flux per unit cell. For $H^\pm$ we assume vanishing on-site potential $V^\pm_n \equiv 0$ and, in order to generate twists, hopping terms $t^{\pm,0} = -t^0$. Fig. 3 corresponds to Fig. 2c, where the three tight-binding bands now show fine structure, while on a coarse scale they display the same twists and flattening as in Fig. 2c. For large $|\lambda|$ the individual spectra of $H^\pm$ and $H^0$ are uncoupled and all eigenfunctions are extended. Surprisingly, in the $\lambda$ region between the twists the intermediate band has localized eigenfunctions only. If for $H^0$ we assume the Anderson model for disordered systems $\overline{\mathbf{W}}$, where $V^0_n$ is a uniform random variable in the interval $[-V^0/2, V^0/2]$, for $\lambda = 0$ we find a decreasing localization length of eigenfunctions as the coupling parameter $\epsilon$ is increased (Fig. 4a, squares). As a third example for $H^0$ we assume the Fibonacci chain model $[17]$, a one-dimensional model for quasicrystals with potential terms taking on the values $V^0$ and $-V^0$ according to a Fibonacci sequence. Remarkably, at $\lambda = 0$ increasing $\epsilon$ lowers the fractal dimension of the energy spectrum (Fig. 4b, squares). These three systems show...
the opposite of what one would expect naively: The
A
for localization length.
participation ratio corresponds to a decreasing (increasing)
theory (Eqs. (5) and (6)). An increasing (decreasing) inver-
sor model with the effective terms $\bar{t}^\pm = 1$ (squares) and $t^\pm = 1$ (diamonds), resp. Solid ($t^\pm = -1$) and
dashed ($t^\pm = 1$) lines are the results for an isolated
Anderson model with the effective terms $V^0_n$ and $t^0$ of perturbation
theory (Eqs. (5) and (6)). An increasing (decreasing) inverse participation ratio corresponds to a decreasing (increasing)
localization length.

b) Same as (a) showing the fractal (box-counting) dimension for $H^0$ representing the Fibonacci model ($V^0 = 1.5$, $t^0 = 1$, $A = 100$).

the opposite of what one would expect naively: The
coupling of a given tight-binding model ($H^0$) to mod-
ells having extended eigenfunctions ($H^\pm$) in these three
cases leads to localization, reduced localization lengths, and reduced fractal dimensions, respectively. How is that possible?

One can try to understand these effects of ABCs in-
tuitively: The reduced width of the intermediate band in
Fig. 2c resulting from subsequent ABCs with twists
 corresponds to reduced hopping terms in a tight-binding
Hamiltonian $H^0$. More generally, one may expect that the ratio of potential terms to hopping terms is increased by these ABCs with twist. This would naturally explain the observed results, as for increasing $V^0/t^0$ the Harper model makes a transition from metal to insulator $[3]$, the Anderson model has a decreasing localization length $[1]$, and the energy spectrum of the Fibonacci model has a decreasing fractal dimension $[13]$.

Further insight can be obtained from a perturbative
 treatment for $\lambda = 0$. By a similarity transformation we obtain $H = S^{-1}HS$, where

$$
S = \begin{pmatrix}
(1 - \epsilon^2/2A^2) & -\epsilon/A & \epsilon^2/2A^2 \\
-\epsilon/A & (1 - \epsilon^2/2A^2) & -\epsilon/A \\
\epsilon^2/2A^2 & \epsilon/A & (1 - \epsilon^2/2A^2)
\end{pmatrix}.
$$

(4)

This choice of $S$ leads to renormalized Hamiltonians $H^\pm_0$ analogous to Eq. (3) that are decoupled order $\epsilon^2/A^2$ for $|V^\pm_0|_{t^\pm_0} \ll A$. The Hamiltonian $H^0$ describing the intermediate band is still triagonal with on-site potential $V^0_n$ and hopping terms $t^0$ up to order $\epsilon^2/A^2$ given by

$$
\bar{V}^0_n = V^0_n (1 - 2\epsilon^2/A^2) + (V^+_n + V^-_n) \epsilon^2/A^2 \\
\bar{t}^0 = t^0 (1 - 4\epsilon^2/A^2).
$$

(5)

For the systems studied above (where $V^+_n = V^-_n = 0$) we find that the ratio $V^0_n/t^0$ is effectively increased by the factor $(1 + 2\epsilon^2/A^2)$. This substantiates the intuitive explanation of the preceding paragraph. E.g., in the Harper model ABCs with twist may induce a transition from extended states ($V^0/t^0 < 2$) to localized states ($V^0/t^0 > 2$). For two subsequent ABCs without twist, i.e. when the hopping terms $t^\pm$ and $t^0$ have the same sign, the above perturbative treatment yields

$$
\bar{V}^0_n = V^0_n (1 - 2\epsilon^2/A^2) + (V^+_n + V^-_n) \epsilon^2/A^2 \\
\bar{t}^0 = t^0 (1 - 4\epsilon^2/A^2).
$$

(6)

instead. Thus, without twists the ratio $V^0/t^0$ effectively decreases by the factor $(1 - 2\epsilon^2/A^2)$. In this case we therefore expect the opposite effects on eigenfunctions and spectrum. Using the renormalized terms of Eqs. (6) and (7) we can compute the localization length for an isolated Anderson model and the fractal dimension $D_0$ for an isolated Fibonacci band. Comparison with the numerical results in Fig. 4a) and b) gives a good agreement and thus confirms our explanation in terms of renormalized tight-binding parameters. In contrast to the case of ABCs with twist, here an intuitive understanding is missing, and one has to rely on the above perturbative treatment. The phenomena associated with ABCs analyzed above also do occur when there is just a single ABC, although in a more complex way. Thus they should be generic for all models with ABCs.

Now we will apply these general results to the well-
studied kicked Harper model (KHM) $[4, 14]$. This model combines the quantum mechanical properties of Harper’s equation with an onset of chaos in classical phase space. It shows similar phenomena $[4, 11]$, as those discussed for ABCs, but they have remained unexplained so far. The KHM is given by the Hamiltonian

$$
H = L \cos p + K \cos x \sum_n \delta (t - n)
$$

(7)

with $p = -ih\partial/\partial x$ and an effective $h$. For small $K$ and $L$ its spectrum is close to the Harper spectrum for $\sigma = h/2\pi$ and $V^0/t^0 = 2K/L$ up to a scaling by a factor proportional to $K$ $[4]$ (Fig. 5). In particular, the spectrum clusters into subbands each of which may be described by a Harper-like model $[5]$. Upon increasing the parameters $K$ and $L$ these subbands make band crossings. As soon as the classical limit is non-integrable (i.e., mixed or fully chaotic) such crossings are avoided. Therefore our general findings on ABCs apply and one may expect all the phenomena discussed above to occur. Indeed, this is the case. For example, for the parameters of Fig. 5 transitions from extended to localized eigenfunctions can...
be observed as were numerically found in Refs. \[3,4\]. They occur along with ABCs, however, in a more complex way than in the simple model system of Eq. (3).

Tuning these metal-insulator transitions necessarily leads to states right at the transition point, which, e.g., in the Harper model correspond to a singular continuous spectrum. We therefore also understand the findings of Borgonovi and Shepelyansky \[15\], that for the dual parameters of Fig. 5 at $K = 4$ and $L = 7$ part of the spectrum seems to be singular continuous \[21\]. Similarly, the increase of the fractal dimension of the spectrum for increasing $K = L$ \[8\] can be understood on the basis of ABCs as analyzed above in the Fibonacci model (Fig. 4b).

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