Piezoelectricity: Quantized Charge Transport Driven by Adiabatic Deformations

J.E. Avron [a*], J. Berger[a] and Y. Last[b]
[a] *Department of Physics, Technion, 32000 Haifa, Israel*
[b] *Division of Physics Mathematics and Astronomy, Caltech, Pasadena, CA 91125*
* e-mail avron@physics.technion.ac.il
(September 18, 1996)

We study the (zero temperature) quantum piezoelectric response of Harper-like models with broken inversion symmetry. The charge transport in these models is related to topological invariants (Chern numbers). We show that there are arbitrarily small periodic modulations of the atomic positions that lead to nonzero charge transport for the electrons.

PACS numbers: 72.10 Bg, 72.20 Mg

The Harper model can be interpreted as a tight-binding quantum Hamiltonian describing the dynamics of non-interacting electrons on a two dimensional lattice in the presence of magnetic fields. It is known to have interesting Hall transport properties. Here we study the electric response of Harper-like models to adiabatic changes in the hopping amplitudes. Changes in the hopping amplitudes have a natural interpretation as elastic deformation of the underlying lattice. As we shall show, such deformations can drive electron transport. We shall refer to this kind of response as piezoelectricity. Like the Hall conductance in the integer Hall effect [1,2], and in quasi-one dimensional systems [3], the Thouless pump [4,5], the Magnus force [6], adiabatic charge transport in networks [7], adiabatic spin transport [8], and adiabatic viscosity [9], it is a transport phenomenon related to the adiabatic curvature and Berry's phases [10].

Let us first summarize the central findings: 1. Harper-like models with broken time reversal and broken inversion symmetry have, in general, nontrivial piezoelectric response. 2. Appropriate *periodic* modulations of the atomic positions lead to integral charge transport given by appropriate Chern integers. This implies that an ac driving has a response with a dc component. 3. There are *arbitrarily small* periodic deformations that transport integral (and nonzero) charges over macroscopic distances. These periodic cycles trap level crossings in parameter space.

The topological significance of piezoelectricity was noted in [9], but vanished for the models considered there (Landau Hamiltonians). Thouless [4] and subsequently Niu [5] constructed one dimensional models of charge pumps where integral charge transport (given by a Chern number) is driven by one periodic potential sliding past another. Here, the model, the driving and the details are different, but the spirit is the same.

We shall focus on a family of Harper models, $H(\vec{t},\vec{k},\eta,\phi)$, which arises from tight binding models associated with a two dimensional triangular lattice. Each site of the lattice has a coordination number six and the basic plaquettes are triangles. Each up-triangle in the lattice is surrounded by three down-neighbors and vice versa. The magnetic flux through the up-triangles is $\phi/2+\eta$ and $\phi/2-\eta$ through the down-triangles. $\phi = 2\pi\ p/q$, with p,q relative primes, and $|\eta| \le \pi/2$ is a measure of the asymmetry in the fluxes through the up/down triangles in units where the quantum of flux is 2π. The hopping amplitudes associated with the three basic vectors of the triangular lattice are $t_j \in \mathbb{R}$, $j = 1,2,3$. The corresponding Harper model is:

$$\left(H(\vec{t},\vec{k},\eta,\phi)\Psi\right)(n) = \left(t_1 + t_3 y_n e^{i\phi/2}\right) x\Psi(n+1)\ + \\ 2t_2\cos(n\phi+k_2)\Psi(n) + \left(t_1 + t_3\bar{y}_n e^{i\phi/2}\right)\bar{x}\Psi(n-1). \quad (1)$$

$x=\exp(ik_1)$, $y_n = \exp i(n\phi+k_2-\eta)$, $\Psi(n+q)=\Psi(n)\in\mathbb{C}$ and $\bar{x},\bar{y}_n$ are the complex conjugates of x, y_n. $\vec{k}$ are Bloch momenta with ranges $|k_1|\le\pi/q$, $|k_2|\le\pi$. The model was introduced in [11] who studied the Hofstadter spectrum in the case $\vec{t}=(1,1,1)$.

The class of models in Eq. (1) is the simplest among Harper-like models with interesting piezoelectric response. The simpler versions of the Harper model and, in particular, the classical Harper model on the rectangular lattice and its generalizations [12], do not have interesting adiabatic piezoelectric response. The reason for this is that inversion symmetry needs to be broken. This is a fact about piezoelectricity that goes back to the brothers Curie [13]. Inversion symmetry is broken if $\eta\ne 0 \bmod \pi$. Inversion symmetry is preserved in the classical Harper model and the generalizations studied in [12].

Let $|\psi(\vec{t},\vec{k},\eta)\rangle$ be a normalized Bloch state of the Harper model in Eq. (1). Consider a closed loop $\gamma\subset\mathbb{R}^3$ in the space of hopping amplitudes. When γ is traversed adiabatically (this, of course, subsumes that the gap remains open), the charge $Q(\gamma,k_2,\eta)$ transported from $-\infty$ to ∞ in the k_1 direction for fixed k_2 channel for each full band is given by [4,7]

$$Q(\gamma,k_2,\eta) = \frac{1}{\pi}\mathrm{Im}\int_{-\pi/q}^{\pi/q} dk_1\ \int_\gamma \langle\frac{\partial\psi}{\partial k_1}|\vec{\nabla}_t\psi\rangle\cdot d\vec{t}. \quad (2)$$

The charge, if well defined, is an integer—a Chern number. The total charge transported by the system is the sum over the relevant k_2 channels and the occupied bands. When the system is an infinite two dimensional crystal then all the k_2 channels are relevant. On the other hand, for a strip of finite width with (possibly twisted) periodic boundary conditions, only a discrete set of values of k_2 contributes. For reasons that shall become clear later, finite strips are the more interesting case.

The difficulties in studying Chern numbers of model Hamiltonians [1,7,9,14] (and this one is no exception) are: First, one needs to establish that the Chern numbers are well defined. For the problem at hand, this means that one needs to isolate a range of parameters k_2, η and ϕ for which the gaps surrounding an energy band remain open when $\vec{t}$ and k_1 run over their full range. Second, the Chern number may be well defined but zero, a case that is not very interesting for transport. For this not to be the case, the surface of integration in Eq. (2) must be protected against contraction. For certain transport properties such as those considered, e.g., in [1,7,8], the surface of integration had such a protection built in. This is not the case here. The cycle of deformations, γ, is a closed orbit in the three dimensional space of deformations, and such an orbit can be contracted to a point. If during this contraction the integrand in Eq. (2) remains continuous, the Chern number is zero. So, for the Chern number to be nonzero, the orbit of deformations γ *must trap level crossing.* Finally, one needs to worry about global questions: $Q(\gamma, k_2, \eta)$ must be well defined for *all* of the relevant k_2 channels and must not sum up to zero. It turns out that the Harper model is rich enough so that everything actually happens there; there are good orbits and parameters where one finds nonzero quantized transport, but also bad ones where various bad things happen.

The Bloch Hamiltonian, Eq. (1), is a homogeneous function of $\vec{t}$ of order one: $H(\vec{t}, \vec{k}, \eta, \phi) = |\vec{t}|\ H(\hat{t}, \vec{k}, \eta, \phi)$. The eigenvectors are independent of $|\vec{t}|$, and the length of $\vec{t}$ therefore does not contribute to Eq. (2). We shall henceforth take $\hat{t}$ to be on the unit sphere. The three additional continuous parameters, $\vec{k}$ and η are angular variables. Eq. (1) depends on five continuous parameters, $(\hat{t}, \vec{k}, \eta)$. The five dimensional parameter space is topologically the product of a two-sphere and a three-torus.

To get one's hands on the Chern numbers for this model, one needs, as we have seen, to have good control over level crossings. One can use symmetry considerations to reduce the study of crossings from the full range of the parameters to a part of the parameter space. Indeed, there are three linear transformations of the parameters which are implemented by either unitary or anti-unitary transformations. These are

$$\{k_j \to k_j + 2\pi/q\}, \quad \{\eta \to -\eta,\ \vec{k} \to -\vec{k}\},$$
$$\{k_1 \to \eta - k_1 - k_2 + (1-(-1)^q)\,\phi/4,\ t_1 \leftrightarrow t_3\} \qquad (3)$$

As a consequence of this, the spectral analysis of $H(\hat{t}, \vec{k}, \eta, \phi)$, can be restricted to the range:

$$-\pi/q \le k_j < \pi/q, \quad 0 \le \eta < \pi/2, \quad t_3 \le t_1. \qquad (4)$$

We shall take t_1 and t_2 to be our coordinates on the sphere of deformations. For the sake of concreteness we restrict ourselves to the positive quadrant $t_j \ge 0$, $j = 1,2,3$, and to the ground state of Eq. (1). We shall call the point on the unit sphere with $t_j = 1$ "the j-th pole."

Let Γ be the set of points where the lowest eigenvalue of Eq. (1) is degenerate. By $\Gamma(k_2 = c)$ we shall denote the restriction of Γ to the subspace with fixed channel $k_2 = c$ and by $\Gamma(k_2 = c, \eta = d)$ we denote the restriction to a fixed channel and asymmetry, etc. Recall that the von Neumann-Wigner rule [15] says that a complex Hermitian matrix which depends on d parameters has, generically, eigenvalue crossings on a surface of dimensions $d-3$. One therefore expects Γ to be two dimensional surfaces, $\Gamma(k_2 = c)$ to be one dimensional curves and $\Gamma(k_2 = c, \eta = d)$ to be isolated points. We shall see that this is a good guide to the behavior of the set of level crossings away from special points, e.g., the poles. For a generic point of $\hat{t}$, the von Neumann-Wigner rule says that $\Gamma(\hat{t})$ is a discrete set of points in $\vec{k} \otimes \eta$ space. At the poles we shall find, instead, that $\Gamma(t_j = 1)$ is a two dimensional surface. Of course, the poles are special points, and the failure of von Neumann-Wigner there is no source of concern.

At the poles Eq. (1) can be diagonalized by hand. At the 2-pole the Hamiltonian is already in a diagonal form. At the 1-pole it is diagonalized by plane waves and at the 3-pole, by plane waves up to an appropriate gauge transformation. The restrictions of Γ to the poles, $\Gamma(t_j = 1)$, can be determined explicitly. More precisely, $\Gamma(t_j = 1)$ is the 2D set of points that obey:

$$\begin{aligned} k_1 &= (1+(-1)^q)\phi/4, && \text{for } j=1; \\ k_2 &= -(1+(-1)^q)\phi/4, && \text{for } j=2; \\ k_1 &= -k_2 + \eta\ + (1-(-1)^q)\,\phi/4, && \text{for } j=3. \end{aligned} \qquad (5)$$

The degeneracies at the 1-pole and the 3-pole are related by symmetry, Eq. (3).

Let us now consider the special cases $q = 1,2,3$: The case $q = 1$ corresponds to $\phi = 0$ and is trivial; the Bloch Hamiltonian has one eigenvalue, no crossing, and no charge transport. The case $q = 2$ (or equivalently, $\phi = \pi$) is already interesting. The Bloch Hamiltonian, Eq. (1) reduces to the basic paradigm for Chern numbers—Berry spin 1/2 Hamiltonian:

$$(t_2 \cos k_2)\,\sigma_3 + (t_1 \cos k_1)\,\sigma_1 + (t_3 \cos(k_1 + k_2 - \eta))\,\sigma_2, \quad (6)$$

with σ_j the Pauli matrices. Since the matrix is traceless, levels cross when it vanishes. This gives Eq. (5) and is all of $\Gamma(k_j)$, provided $k_j \ne \pi/2$. At these special points $\Gamma(k_2 = \pi/2)$ is the two great circles $t_1 = 0$ and $t_3 = 0$; similarly, $\Gamma(k_1 = \pi/2)$ is the two great circles $t_2 = 0$ and $t_3 = 0$. If $k_1 = k_2 = \eta = \pi/2$, then the whole unit sphere $|\hat{t}| = 1$ belongs to Γ.

Now that the set of level crossings is known, we can describe the Chern numbers. By the general principles mentioned before, interesting Chern numbers arise when the orbit in deformation space γ traps level crossings. Let γ_j denote a small closed orbit around the j-th pole. For $k_2 \neq \pi/2$ these orbits trap level crossings and are such that the Chern number, Eq. (2), is well defined. The charge transport can be computed by a formula of [16,7]:

$$\begin{aligned} Q(\gamma_1, k_2, \eta) &= \mp \mathrm{sgn}(\cos k_2)\, \mathrm{sgn}(\sin(k_2 - \eta)), \\ Q(\gamma_2, k_2, \eta) &= 0, \\ Q(\gamma_3, k_2, \eta) &= \pm \mathrm{sgn}(\cos k_2)\, \mathrm{sgn}(\sin \eta). \end{aligned} \tag{7}$$

The overall sign depends on the orientation of γ_j, and is opposite for the top/bottom bands. The Chern numbers change (discontinuously) on Γ so the direction of charge transport can be flipped by tuning k_2 and η.

For $k_2 = \pi/2$, the Chern number $Q(\gamma_2, k_2, \eta)$ is not well defined since there are level crossings on the surface of integration. The *total* charge transport is a well defined integer if $k_2 = \pi/2$ is not an allowed channel, and is ill defined if this channel is allowed. For finite strips *with periodic boundary conditions*, odd strips have $k_2 \neq \pi/2$ and the total charge transport is integral. Even strips, and also the infinite two dimensional lattice, include the $k_2 = \pi/2$ channel and do not have a well defined (total) Chern number. For finite strips where the channel $k_2 = \pi/2$ is excluded, the total transport can be read off from Eq. (7). In particular, with maximal breaking of inversion symmetry, $\eta = \pi/2$, an orbit of deformations γ_1 about the 1-pole, transports $\#\{k_2 \text{ channels}\}$ charges in the ground state. The total charge transport is therefore a nonzero integer for any strip (where the number of k_2 channels is finite) and can be arbitrarily large. This shows that summation over the k_2 channels does not cancel in general: in this case, they add. In contrast, for an orbit of deformations γ_3 around the 3-pole, the total charge transport is ± 1 for all odd strips. This is because the allowed values of k_2 are equally spaced and then $\sum \mathrm{sgn}(\cos k_2) = \pm 1$.

We see from this that: 1. The Harper model, Eq. (1), has nontrivial piezoelectric response. 2. For appropriate values of parameters and orbits, the charge transport is given by nonzero Chern integers. 3. The Chern numbers can sum to nonzero integers when summation over channels is taken. 4. Integer transport occurs also for arbitrarily small deformations γ.

One may criticize the $q = 2$ example of piezoelectric response as being too special in that the deformations γ that give charge transport are about points in parameter space where two hopping amplitudes vanish. This is a rare event, analogous to multicriticality. Can one have piezoelectric transport also if all hopping amplitudes remain positive? As we shall see, this happens for the Harper model with $q = 3$. The price we shall pay is that the analysis of the set of level crossing is more complicated and part of it relies on detailed numerical analysis.

For $q = 3$, the model is described by a 3×3 matrix with the characteristic polynomial

$$\begin{aligned} E^3 - 3E = 2h(\hat{t}, \vec{k}, \eta) = t_1^3 \cos 3k_1 + \\ t_2^3 \cos 3k_2 - t_3^3 \cos\left(3(k_1 + k_2 - \eta)\right) + 3t_1 t_2 t_3 \cos(\eta). \end{aligned} \tag{8}$$

Eq. (8) is a strong version of Chamber's relation: the coefficients of E are not only independent of $\vec{k}$, but also of $\hat{t}$ and η. Therefore, the band edges are at extrema of h in the entire five-dimensional parameter space. The set of curves where the first gap closes for $q = 3$ is obtained when $E = -1$ and $h = 1$.

The strategy we use to get hold of the degeneracy surface Γ is the following: At the 1-pole, Eq. (5) gives a two dimensional planar piece of Γ. (This two dimensional plane projects to a line in Fig. 1.) The line $\Gamma(t_1 = 1, \eta = 0)$ turns out to be a line of self-intersection of Γ. One two dimensional piece is given in Eq. (5). The intersecting two dimensional piece can be obtained as follows. Pick any point on $\Gamma(t_1 = 1, \eta = 0)$ and expand h in powers of t_2 and require that $h = 1$ to every order. If we now use k_2 and t_2 as the parametric representation of Γ we find:

$$\begin{aligned} k_1 &= \sin(3k_2) t_2^3/3 + \sin(3k_2) t_2^5 + \ldots \quad ; \\ t_1 &= 1 - t_2^2 + \cos(3k_2) t_2^3 + \ldots \quad ; \\ \eta &= -\sin(3k_2) t_2 - \sin(6k_2) t_2^2/2 + \ldots \quad . \end{aligned} \tag{9}$$

In this parametric representation, t_2 is small and k_2 is arbitrary. This gives us a thin strip of Γ, which intersects that of Eq. (5). We can extend this strip using the fact that the tangent plane to Γ is the kernel of the Hessian of h. In other words, with k_2 fixed, the curve of degeneracy, $\Gamma(k_2)$, may be described as the solution of an ordinary differential equation: The velocity in parameter space is given by the kernel of the Hessian of h. Near the 3-pole, $\Gamma(k_2)$ is given by (9) and (3).

Several curves describing degeneracies are shown in the figure. We chose t_1 and t_2 as our coordinates on $\hat{t}$ restricted to the positive quadrant, $0 \leq t_j \leq 1$. Let us denote by Γ_c the degeneracy surface with the poles excised. The tongue-like curves in Fig. 1 are $\Gamma_c(k_2 = -\pi/18)$ and $\Gamma_c(k_2 = -\pi/3)$. By the von Neumann-Wigner rule one expects these to be one dimensional curves, and indeed they are. For the orbit of deformation γ shown in this figure, that is, a small circle centered at $t_1 = 0.355, t_2 = 0.446$, the charge transport is $Q(\gamma, -\pi/18, \pi/9) = \pm 1$ (the sign depends on the orientation on which γ is traversed). This gives an example where a Chern number is nonzero for a small orbit of deformations that lies entirely in the positive quadrant of hopping amplitudes.

For $q = 2$, we have seen that Chern numbers for the infinite crystal included channels with ill defined Chern numbers. One may wonder if this is also the case for $q =$

3. The answer is no. For $q=3$, all sufficiently small paths γ_j around the poles have well defined Chern numbers for *all* k_2 channels, and some of these are nonzero. It is easy to verify this for $\eta=\pi/2$ where one can check that all of Γ is at the poles. More is true; Γ is in fact restricted to the poles for all $\pi/6<\eta\le\pi/2$. One way to see this, is by analysis at the vicinity of the point $\hat{t}=1/\sqrt{3}(1,1,1)$, $\vec{k}=-\pi/18(1,1)$, $\eta=\pi/6$. One finds that η attains its maximum value on Γ_c at this point. Further study shows that, in fact, for all $\eta\ne 0 \bmod \pi$ a sufficiently small orbit γ_j about the j-pole avoids Γ. The Chern numbers for these orbits γ_j are all well defined, and by numerical integration we found $Q(\gamma_j,k_2,\eta)=\pm1,0,\mp1$ for $j=1,2,3$ pole respectively, for all k_2 channels and $\eta\ne 0$.

In conclusion: we have described a method for analyzing the Chern numbers that arise in inversion asymmetric Harper models and have found explicit situations with nonzero quantized piezoelectric response. In all these cases nonzero transport occurs for arbitrarily small orbits, and this can happen also when all the hopping amplitudes are positive.

We thank A. Auerbach and P. Zograf for discussions and E. Akkermans for bringing ref. [3] to our attention. This work is supported in part by GIF, the Israel Science Foundation, the DFG and by the Fund for the Promotion of Research at the Technion. YL acknowledges the hospitality of ITP at the Technion and JA the hospitality of Caltech.

[1] D.J. Thouless, M. Kohmoto, P. Nightingale and M. den Nijs, Phys. Rev. Lett. **49**, 40 (1982).
[2] M. Stone, Editor, *The Quantum Hall Effect*, World Scientific, Singapore (1992); R. E. Prange and S .M. Girvin, *The Quantum Hall Effect* , Springer (1987); J. Bellissard, A. van Elst, H. Schultz-Baldes, J. Math. Phys. **35** 5373 (1994); D.J. Thouless, J. Math. Phys. **35**, 1–11 (1994); R. Seiler, in *Recent developments in Quantum Mechanics*, A. Boutet loop Monvel et. al. Eds., Kluwer, Netherland (1991); H. Kunz, Comm. Math. Phys. **112**, 121 (1987).
[3] D. Poilblanc, G. Montambaux, M. Heritier and P. Lederer, Phys. Rev. Let. **58**, 270 (1987); V.M. Yakovenko, Phys. Rev. B **43**, 11353–11366 (1991); Q. Niu, Phys. Rev. B **49**, 13554–13559 (1994).
[4] D.J. Thouless, Phys. Rev. B **27**, 6083 (1983).
[5] Q. Niu, Phys. Rev. Lett. **64**, 1812 (1990).
[6] D.J. Thouless, P. Ao and Q. Niu, Phys. Rev. Lett. **76**, 3758–3761 (1996).
[7] J.E. Avron, A. Raveh and B. Zur, Rev. Mod. Phys. **60**, 873 (1988); J.E. Avron and L. Sadun, Ann. Phys. **206**, 440–493 (1991); J.E. Avron, R. Seiler and P. Zograf, Phys. Rev. Lett. **73**, 3255–3257 (1994).
[8] F.D.M. Haldane and D. Arovas, Phys. Rev. B **52**, 4223–4225 (1995); G.E. Volovik and V.M. Yakovenko, J. Phys. Cond. Mat. **1**, 5263–5274 (1989);
[9] J.E. Avron, R. Seiler and P. Zograf, Phys. Rev. Lett. **75**, 697–700 (1995).
[10] M.V. Berry, Proc. Roy. Soc. A **392**, 45–57 (1984); A. Shapere, F. Wilczek, *Geometric Phases in Physics*, World Scientific, Singapore, 1989.
[11] J. Bellissard, Ch. Kreft and R. Seiler, J. Phys. A **24**, 2329–2353 (1991).
[12] J.H. Han, D.J. Thouless, H. Hiramoto and M. Kohmoto, Phys. Rev. B **50**, 11365–11380 (1994-II).
[13] W.G. Cady, "Piezoelectricity", McGraw-Hill, 1946.
[14] S.P. Novikov, Sov. Math. Dokl. **23**, 298–303 (1981); P. Leboef, J. Kurchan, M. Feingold, D. Arovas, Phys. Rev. Lett. **65**, 3076 (1990).
[15] J. von Neumann and E. Wigner, Phys. Z. **30**, 467–470 (1929).
[16] B. Simon, Phys. Rev. Lett. **51**, 2167–2170 (1983).

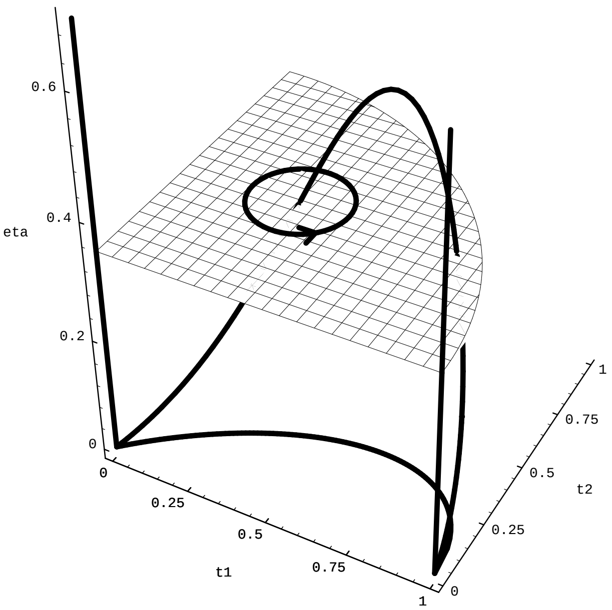

FIG. 1. Curves on which the first gap closes for $q=3$. The vertical axis is the asymmetry flux η. The horizontal plane is the positive quadrant in the plane $0\le t_1,t_2\le 1$, $t_1^2+t_2^2\le 1$. The hatched region is this positive quadrant at $\eta=\pi/9$. The two vertical lines at $t_2=0$ correspond to the gap closure in Eq. (5). The tongue-like curve is the line of gap closure at $k_2=-\pi/18$. It links with a small circle γ in the hatched plane, centered at $(t_1=.355,t_2=.446)$. A periodic deformation along γ transports a unit of charge. The curve in the plane $\eta=0$ is the line of gap closure for $k_2=-\pi/3$.