Chem Numbers and Adiabatic Transport in Networks with Leads

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We study the Chem numbers associated with the adiabatic conductances of mesoscopic systems with leads. We describe the results of exact calculations of all the Chem numbers of several model networks. For a network with one lead we find the integer conductances $0, \pm 1$. For a network with three leads we find noninteger conductances bounded by 1.

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It is known¹ that the adiabatic conductances of quantum systems can, in certain cases, be identified with the adiabatic curvature associated with Berry's phase.² Quantized conductances are then the first Chem number—the integer obtained by averaging the adiabatic curvature. For this reason, the computation of Chem numbers for Schrödinger operators is an interesting physical problem.

The Chem numbers of noninteracting electrons in a magnetic field and periodic or quasiperiodic potentials have been studied extensively.³ They satisfy Diophantine equations, and can be very large for suitable fields. Chem numbers have also been studied in the context of localization theory.⁴ The motivation for much of this comes from the quantum Hall effect.

Another setting where Chem numbers have been studied is for several relatively simple mesoscopic networks.⁵ These networks may be represented by graphs (e.g., Fig. 1). The loops are threaded by independent, externally controllable, flux tubes ϕ_i , $i = 1,2,3$. The electrons are constrained to the links.

One is interested in the charge transported around loop *i* as the flux ϕ_i increases adiabatically by the unit of quantum flux, which we take to be 2π . This charge may depend on ϕ_i (and on the remaining flux ϕ_k), and need

FIG. l. (a) A network with three loops threaded by three independent flux tubes, with six links of equal length meeting at three vertices. (b) The network of (a) with three long leads of length I emanating from the vertices. (c) The network of (a) with one long lead of length I emanating from a vertex.

not be an integer. However, this charge averaged over ϕ_i is an integer, provided the corresponding eigenstate is nondegenerate for all ϕ_i and ϕ_j . This integer, a Chern number, labels the eigenstate bundle. It generally is an antisymmetric and periodic function of the third flux ϕ_k , with discontinuities at the values of ϕ_k where level crossings occur.

Our purpose here is to initiate the study of Chem numbers for mesoscopic networks with long tails (e.g., leads), similar to those in Figs. 1(b) and 1(c). Leads play a significant role in mesoscopic systems.⁶ In the present context, with leads to length l , there are $O(l)$ eigenstates in each energy interval, and so there are many Chem numbers to compute. This poses the following interesting theoretical problems:⁷ (a) What is the distribution of these Chem numbers? (b) Is the charge transport quantized to be an integer in the $l \rightarrow \infty$ limit? (c) Can one get arbitrarily large Chem numbers? (d) What is the dependence on the Fermi energy? (e) How are networks with and without leads related?

In this Letter we address these questions for models associated with the graphs in Fig. 1. Lack of space prevents us from describing the detailed analysis, but we shall outline the main ideas. Details and additional results will be presented elsewhere.

The Schrödinger equation for noninteracting electrons associated with the graphs in Fig. ¹ reduces to the study of a 3×3 matrix problem. The construction of such matrices has been described in Refs. 5 and 8. We take all the short links to be of length 1, and all the leads to be of identical length $l \gg 1$. For these graphs the relevant matrices are

$$
H^{(j)}(k,\phi) = -\left[\sin(k)\right]^{-1} \begin{bmatrix} \lambda_i^{(j)} & 1+z & 1+\bar{y} \\ 1+\bar{z} & \lambda_2^{(j)} & 1+x \\ 1+y & 1+\bar{x} & \lambda_3^{(j)} \end{bmatrix}, \quad (1)
$$

where j labels the model $(a, b, or c)$ and

$$
x \equiv \exp(i\phi_1), y \equiv \exp(i\phi_2), z \equiv \exp(i\phi_3).
$$
 (2)

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For model a we have

$$
\lambda_1^{(a)} = \lambda_2^{(a)} = \lambda_3^{(a)} = -4\cos(k) , \qquad (3)
$$

for model *b* we have

$$
\lambda_1^{(b)} = \lambda_2^{(b)} = \lambda_3^{(b)} = -4\cos(k) + \sin(k)\tan(kl), \quad (4)
$$

and for model c we have

$$
\lambda_1^{(c)} = \lambda_2^{(c)} = -4\cos(k),
$$

\n
$$
\lambda_3^{(c)} = -4\cos(k) + \sin(k)\tan(k),
$$
\n(5)

The energy of the particle is $k^2/2m$, $k > 0$, and the null space of $H^{(j)}(k, \phi)$ gives the vector of amplitudes of the wave function at the vertices of the graph. The explicit matrix in (1) involves a choice of gauge and a choice of scattering potentials at the vertices.

In the following we take l to be an integer. This makes $H^{(j)}(k, \phi)$ periodic in k and in each component of ϕ , with period 2π , and so we can restrict our attention to one period. Model a has no leads, but we give the results because they are needed for models b and c below.

Model *a*: $H^{(a)}(k, \phi)$ depends only on cos(*k*) and ϕ , so it is sufficient to consider the interval $0 \le k \le \pi$ only. At fixed ϕ , there are three eigenstates in this interval (and another three in the interval $\pi \leq k \leq 2\pi$). Label the levels 1, 2, and 3 in increasing order of energy. To compute the Chem numbers of the three levels one has to identify the points in $(cos(k), \phi)$ space where levels cross. With each such crossing an integer "charge" is associated, which gives the discontinuity of the Chem number as the degeneracy is crossed. The Chem numbers are then determined by adding the charges between 0 and ϕ_3 .⁵

There are four points of level crossing, each lying on the body diagonal $\phi_1 = \phi_2 = \phi_3$. We write [ij] for a crossing between levels i and j , and $[123]$ for a crossing of all three levels. Then these crossings occur at

$$
[12] \pm = (\cos(k) = \frac{1}{4}, \phi_1 = \phi_2 = \phi_3 = \pm 2\pi/3),
$$

\n
$$
[123] = (\cos(k) = 0, \phi_1 = \phi_2 = \phi_3 = \pi),
$$

\n
$$
[23] = (\cos(k) = -\frac{1}{2}, \phi_1 = \phi_2 = \phi_3 = 0).
$$

\n(6)

The associated charges are

$$
ch([12]_{\pm}) = -1, ch([123]) = 2, ch([23]) = -2. (7)
$$

The behavior near $[12]_+$ is approximated by the 2×2 spin Hamiltonian $H = -(\delta \phi) \cdot \mathbf{j}$ with $J = \frac{1}{2}$, and near [123] by the 3×3 Hamiltonian $H = +(\delta \phi) \cdot J$ with $J=1$. Near [23] the Hamiltonian is not adequately described by a linearization; higher-order expansions are needed to compute the charge.

We write $g_{12}(j, \phi_3)$ for the 1-2 Chern number as a function of ϕ_3 for level j. g_{12} is periodic in ϕ_3 with period 2π , and, by time reversal $g_{12}(j,\phi_3) = -g_{12}(j, -\phi_3)$, and so we need only compute g_{12} for $0 \le \phi_3 \le \pi$. We find

$$
g_{12}(1,\phi_3) = g_{12}(6,\phi_3) = \begin{cases} 0, & \text{for } 0 < \phi_3 < 2\pi/3 \\ 1, & \text{for } 2\pi/3 < \phi_3 < \pi \end{cases},
$$

$$
g_{12}(2,\phi_3) = g_{12}(5,\phi_3) = \begin{cases} 1, & \text{for } 0 < \phi_3 < 2\pi/3 \\ 0, & \text{for } 2\pi/3 < \phi_3 < \pi \end{cases},
$$
 (8)

$$
g_{12}(3,\phi_3) = g_{12}(4,\phi_3) = -1
$$
, for $0 < \phi_3 < \pi$.

By rotational symmetry g_{23} and g_{31} are similar (as functions of ϕ_1 and ϕ_2 , respectively, instead of ϕ_3).

Model *b*: There are $6l+6$ energy levels in a basic period $0 \le k \le 2\pi$. However, under rescaling of the energy axis the model is equivalent to $1 + 1$ copies of model a —the only difference between a and b being the functional dependence of λ and k in Eqs. (3) and (4). The Chem numbers are given by Eq. (8), except that the first triplet (1,2,3) repeats itself $l+1$ times in the interval $0 \le k < \pi$, while the second triplet (4,5,6) repeats itself $l+1$ times in the interval $\pi \le k < 2\pi$. $0 \le k \lt \pi$, while the second triplet (4,5,6) repeats itself

The periodic repetition of Chem numbers on small energy scales leads to real (i.e., noninteger) transport. To see this, let $P(k) = \{1 + \exp[\beta(k^2 - k_f^2)/2m]\}^{-1}$ be the Fermi-Dirac distribution with $\pi^2/ml^2 \ll \beta^{-1} \ll \pi^2/m$ and k_F in $(0,\pi)$. Then, with $g_{12}(j,\phi_3)$ the Chern number of level j , we have

$$
\langle g_{12}\rangle(\phi_3, \beta) \equiv \sum_j P(E_j)g_{12}(j, \phi_3)
$$

= $g_{12}(1, \phi_3)\omega_{13} + g_{12}(2, \phi_3)\omega_{23}$
= $\begin{cases} \omega_{23}, \text{ for } 0 < \phi_3 < 2\pi/3 \\ \omega_{13}, \text{ for } 2\pi/3 < \phi_3 < \pi, \end{cases}$ (9)

where $\omega_{13}(\phi_3)$ and $\omega_{23}(\phi_3)$ are weights, $0 < \omega_{23}$ $< \omega_{13} < 1$. Specifically, $\omega_{ij} (\phi_3)$ is the difference in the probability $P(k)$ between levels i and j, divided by the probability difference between successive copies of level i. Although these differences vary with k , their ratio does not, at least in the $l \rightarrow \infty$ limit. These weights in general depend on ϕ_3 . The 1-2 conductance is then bounded by 1, and is discontinuous at $\phi_3 = 0, \pm 2\pi/3, \pi$.

Model c : There is an eigenstate at each interval of approximate size π/l of the k axis, and so in the basic period 2π there are $O(2l)$ eigenstates. To locate the charges we introduce some terminology.

The singular set of the third vertex is the set of points in (k, ϕ) space where the minors of $H^{(c)}(k, \phi)$ with respect to the third row all vanish. That is, the set

$$
[4\cos(k)]^2 = (1+z)(1+\bar{z}),
$$

\n
$$
-4\cos(k)|1+y|^2 = (1+x)(1+y)(1+z).
$$
 (10)

Since at a level crossing the Hamiltonian $H^{(c)}(k, \phi)$ has rank at most 1, all the level crossings (and so all the

charges) must lie on the singular set. This set is composed of three one-dimensional "strings" $S₁, S₁₁,$ and S_{III} , and one two-dimensional "sheet" S_H , given by the formulas

$$
S_1: x = \bar{y}, z = 1, \cos(k) = -\frac{1}{2},
$$

\n
$$
S_{11}: x = y, z = x^{-2}, \cos(k) = -\cos(\phi_1)/2,
$$

\n
$$
S_{111}: x = y = -1, \cos(k) = \pm \cos(\phi_3/2)/2,
$$

\n
$$
S_H: z = -1, \cos(k) = 0.
$$
\n(11)

The sheet and S_1 lie on a constant energy surface and support only isolated level crossings (that is, the number of crossings does not grow with *l*). As long as $cos(k_F)$ does not equal 0 or $-\frac{1}{2}$ these crossings do not contribute to the total conductance.

The number of crossings that accumulate on strings S_{II} and S_{III} , on the other hand, is $O(l)$, and their distribution is uniform in k. In every k interval of size π/l there are two crossings on each string. On S_{II} the crossings all have charge -1 , while on S_{III} they all have charge +1.

Consider now the total conductance, which is the sum of the Chem numbers of all the states below a fixed Fermi momentum k_F . This is determined by the charges at the Fermi surface (the charges below the Fermi surface only serving to exchange Chem numbers among the filled states without changing the total). If $0 < k_F < \pi/3$, or $2\pi/3 < k_F < 4\pi/3$, or $5\pi/3 < k_F < 2\pi$, the Fermi surface does not intersect any of the strings, and so all the conductances vanish. If, on the other hand, $\pi/3$ k_F < 2 $\pi/3$, or $4\pi/3 < k_F$ < 5 $\pi/3$, then the Fermi surface slices S_{II} at the two points $\pm \xi$ in flux space and slices S_{III} at the two points $\pm \eta$ in flux space, where

$$
\xi = (\alpha, \alpha, -2\alpha), \quad \eta = (\pi, \pi, -2\alpha),
$$

$$
\cos(\alpha) = -2\cos(k_F).
$$
 (12)

Since $\pm \eta$ (with charge +1) and $\pm \xi$ (with charge –1) have the same values of ϕ_3 , it follows that g_{12} vanishes for all values of ϕ_3 . However, since the second components of η and ξ differ, g_{13} is given by

$$
g_{13}(\phi_2, k_F) = \begin{cases} 0, & \text{for } 0 < \phi_2 < \alpha, \\ 1, & \text{for } \alpha < \phi_2 < \pi. \end{cases}
$$
 (13)

In this case, the average charge transport is an integer.

To sum up, in model a there are six states with $k < 2\pi$, and all six carry integer conductances g_{12} , which are nonzero for some ranges of ϕ_3 . The conductances add up to zero, and so if all states are occupied there is no charge transport, but if only some states are occupied then an integer nonzero total conductance may be observed.

In model b there are $O(l)$ states with $k < 2\pi$, all of which may have nonzero Chem numbers. These states come in triplets, the Chem numbers of each triplet adding to zero. Thus the average conductance gets a contribution only from the slight difference in occupation probability of the states in each triplet. Summing over triplets, this gives the non-integer total conductance of Eq. (9).

In model c there are $O(l)$ states with $k < 2\pi$. Most states may have nonzero Chern numbers for ϕ_3 in some interval of size $O(l^{-1})$, but for any given value of ϕ_3 only a handful $[O(1)]$ have nonzero Chern numbers. These are the states that intersect the singular set at that given value of ϕ_3 (or ϕ_2 for g_{13}). The total conductance is thus always a small integer, and depends on which of these few states are occupied, i.e., how the Fermi energy relates to the energy of these states. The conductance g_{12} is always zero, as states with Chern numbers $+1$ and -1 always occur at the same energy. The conductance g_{13} , however, can be 0, +1, or -1, depending on ϕ_2 and k_F .

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