Adiabatic particle pumping and anomalous velocity

November 17, 2015

Literature:

1. J. K. Asbóth, L. Oroszlány, and A. Pályi, arXiv:1509.02295
2. D. Xiao, M-Ch Chang, and Q. Niu, Rev. Mod. Phys. **82**, 1959.

SSH model, adiabatic evolution, Chern number

A couple of the ideas discussed on previous occasions will be combined.

i) Su-Schrieffer-Heeger (Rice-Mele) model
ii) Adiabatic evolution of eigenstates
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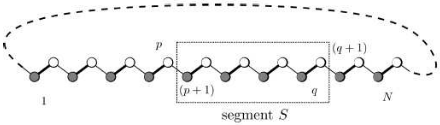

Figure : A segment of the periodic SSH model.

Overview

1) Model system
2) Particle current and group velocity
3) Quasi adiabatic time evolution
4) Pumped current and Berry curvature
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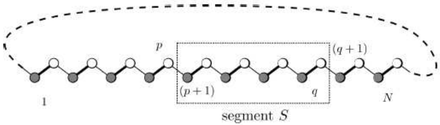
Model system



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Rice-Mele model

$$\hat{H}(t) = v(t)\sum_{m=1}^{N} |m,B\rangle\langle m,A| + h.c.) + w(t)\sum_{m=1}^{N-1}(|m+1,A\rangle\langle m,B| + h.c.)$$
$$+u(t)\sum_{m=1}^{N}(|m,A\rangle\langle m,A| - |m,B\rangle\langle m,B|)$$

Model system

Because of spatial periodicity, the eigenstates are Bloch wave functions. The instantaneous eigenstates read $|\Psi_{n,k}(t)\rangle = |k\rangle \otimes |u_n(k,t)\rangle$, where $n = 1, 2$ are the two bands, k wavenumber.

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and $|u_n(k,t)\rangle$ satisfy the instantaneous Schrödinger equation

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Note, that this is a **different convention** regarding $|u_n(k,t)\rangle$ than what we used the last time to define the Bloch wave functions.

Nevertheless, it is true that $|\Psi_{n,k}(r+R_l)\rangle = e^{ikR_l}|\Psi_{n,k}(r)\rangle$

Model system

We assume that the Hamiltonian is also periodic in time, therefore

1. $\hat{H}(k + 2\pi, t) = \hat{H}(k, t)$
2. $\hat{H}(k, t + T) = \hat{H}(k, t)$, and $\Omega = 2\pi/T$.

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We can rewrite the problem using the following notation. The Hamiltonian is given by (two-band insulator model):

$$\hat{H}(\mathbf{d}(k,t)) = d_x\sigma_x + d_y\sigma_y + d_z\sigma_z = \mathbf{d}\cdot\sigma$$

The parameter vector $\mathbf{d}(k,t)$ reads:

$$\mathbf{d}(k,t) = \begin{pmatrix} \nu + \cos\Omega t + \cos k \\ \sin k \\ \sin\Omega t \end{pmatrix} \Longleftrightarrow \begin{array}{c} v(t) = \nu + \cos\Omega t \\ w(t) = 1 \\ u(t) = \sin\Omega t \end{array}$$

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Influx of particles into a segment

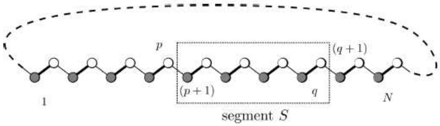

Figure : A segment of the periodic SSH model.

The number of particles $\mathcal{N}_S$ in segment S is given by the expectation value of the operator

$$\hat{\mathcal{N}}_S = \sum_{m \in S} \sum_{\alpha \in \{A,B\}} |m, \alpha\rangle\langle m, \alpha|$$

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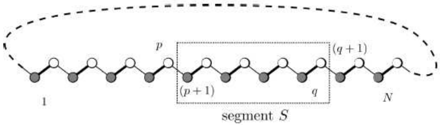

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Due to the time-dependence, the number of particles in a given region changes.

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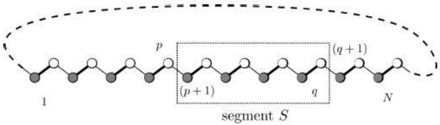

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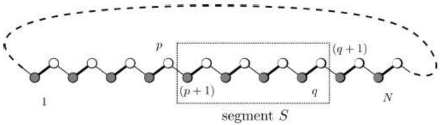

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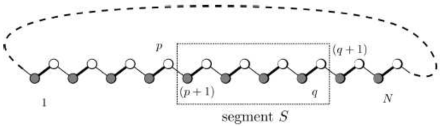
One finds

$$\begin{aligned} \hat{j}_S(t) &= -iw(t)\left[|p+1, A\rangle\langle p, B| - |p, B\rangle\langle p+1, A|\right. \\ &+ \left.|q, B\rangle\langle q+1, A| - |q+1, A\rangle\langle q, B|\right] \end{aligned}$$

Particle current operator



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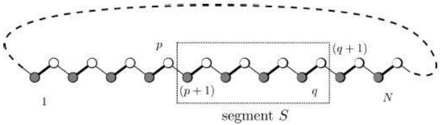

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$$\begin{aligned}\hat{j}_S(t) &= -iw(t)\,[|p+1,A\rangle\langle p,B| - |p,B\rangle\langle p+1,A| \\ &+ |q,B\rangle\langle q+1,A| - |q+1,A\rangle\langle q,B|]\end{aligned}$$

The particle number can change through the interface at $m = p$ and through the interface at $m = q$.
One can define

$$\hat{j}_{m+1/2}(t) = -iw(t)\,(|m+1,A\rangle\langle m,B| - |m,B\rangle\langle m+1,A|)$$

which is interpreted as the **operator describing the net particle flow** through the cross-section at $m + 1/2$.

Particle current and group velocity

Remember: the instantaneous eigenstates read $|\Psi_{n,k}(t)\rangle = |k\rangle \otimes |u_n(k,t)\rangle$ where

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{imk} |m\rangle \qquad m \,:\, \text{site index}$$

and

$$|u_n(k,t)\rangle = a_n(k,t)|A\rangle + b_n(k,t)|B\rangle$$

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We can calculate the diagonal matrix elements of the current operator

$$\langle \Psi_{n,k}(t)|\hat{j}_{m+1/2}(t)|\Psi_{n,k}(t)\rangle = \langle u_n(k,t)|\hat{j}_{m+1/2}(k,t)|u_n(k,t)\rangle$$

where

$$\hat{j}_{m+1/2}(k,t) = \frac{1}{N} \begin{pmatrix} 0 & -iw(t)e^{-ik} \\ iw(t)e^{ik} & 0 \end{pmatrix}$$

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We can recognize that

$$\hat{j}_{m+1/2}(k,t) = \frac{1}{N}\partial_k \hat{H}(\mathbf{d}(k,t))$$

$\Longrightarrow$ the momentum diagonal elements of the current operator are related to the momentum-space Hamiltonian.

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This is a very general result. It applies not only to the Rice-Mele problem but to time-independent problems defined on a lattice and can be generalized to (quasi) two dimensional case (Büttiker formalism etc.)

Particle current and group velocity

Matrix elements of the current operator: in terms of the instantaneous eigenvalues

$$\begin{aligned}\langle u_n(k,t)|\hat{j}_{m+1/2}(k,t)|u_n(k,t)\rangle &= \frac{1}{N}\langle u_n(k,t)|\partial_k \hat{H}|u_n(k,t)\rangle \\ &= \frac{\partial_k E(k,t)}{N} = \frac{v_n(k,t)}{N}\end{aligned}$$

Here $v_n(k,t)$ is the instantaneous *group velocity* of the eigenstate.

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Time evolution governed by quasi-adiabatic Hamiltonian

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Remarks

i) due to the spatial periodicity, the wave number k remains a good quantum number. Therefore we consider the time evolution of a set of two-level system, each labelled by a different k

ii) basically, we are going to use time dependent perturbation theory to calculate the time evolution of the eigenstates

Time evolution governed by quasi-adiabatic Hamiltonian

Quasi adiabatic: for the driving Ω it is fulfilled that $\Omega \ll \Delta E$ where $\Delta E = \min_{\forall k,t,t\to T}(E_2(k,t) - E_1(k,t))$.

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We are looking for the solutions of the following time dependent Schrödinger equation.

$$i\hbar \frac{\partial}{\partial t} |u(t)\rangle = \hat{H}(t)|u(t)\rangle$$

One can expand the wave function in terms of the instantaneous eigenstates of $\hat{H}(t)$

$$|u(t)\rangle = \sum_n \exp\left(-\frac{i}{\hbar}\int_0^t dt' E_n(t')\right) a_n(t)|u_n(t)\rangle$$

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The coefficients satisfy

$$\partial_t a_n(t) = -\sum_l a_l(t)\langle u_n(t)|\partial_t|u_l(t)\rangle \exp\left(-\frac{i}{\hbar}\int_0^t dt'[E_l(t') - E_n(t')]\right)$$

Time evolution governed by quasi-adiabatic Hamiltonian

It is convenient to impose the *parallel transport gauge*. This fixes the phases of the instantaneous eigenstates $|u_n(t)\rangle$ such that

$$\langle u_n(t)|\partial_t|u_n(t)\rangle = \partial_t \mathbf{d}(t)\langle u_n(t)|\frac{\partial}{\partial \mathbf{d}}|u_n(t)\rangle = 0.$$

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If $\partial_t \mathbf{d}(t) \to 0$ then in zeroth order

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If the system is initially in the *n*th eigenstate then approximately it will stay in that eigenstate $\Longrightarrow$ adiabatic theorem.

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First order corrections:
Initially, $a_n(t=0)=1$ and $a_{n'\neq n}(t=0)=0$.
The equation for $a_{n'\neq n}$:

$$\partial_t a_{n'} = -\langle u_{n'}(t)|\partial_t|u_n(t)\rangle \exp\left(-\frac{i}{\hbar}\int_0^t dt'[E_n(t')-E_{n'}(t')]\right)$$

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The approximate solution, up to first order in $\partial_t \mathbf{d}(t)$ is then

$$a_{n'} = -\frac{\langle u_{n'}(t)|\partial_t|u_n(t)\rangle}{E_n - E_{n'}} i\hbar \exp\left(-\frac{i}{\hbar}\int_0^t dt'[E_n(t') - E_{n'}(t')]\right)$$

Time evolution governed by quasi-adiabatic Hamiltonian

Let us now go back to the Rice-Mele model (two-levels).
The time evolution of the lower energy state (ground state) in terms of the instantaneous eigenstates $|u_{1,2}(t)\rangle$

$$|\tilde{u}_1(t)\rangle = e^{-i\int_0^t dt' E_1(t')}\left[|u_1(t)\rangle + i\frac{\langle u_2(t)|\partial_t|u_1(t)\rangle}{E_2(t)-E_1(t)}|u_2(t)\rangle\right]$$

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In the case of cyclic change of parameters, the final state $|\tilde{u}_1(t=T)\rangle$ may differ from the initial state $|u_1(t=0)\rangle$ by a phase factor $e^{i\gamma_1}$ (Berry phase).

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Pumped probability current and Berry curvature

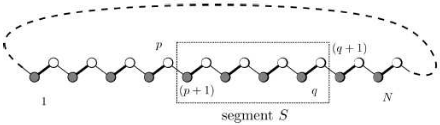
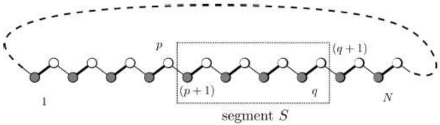


Figure : A segment of the periodic SSH model.

We want to calculate the number of particles $\mathcal{N}$ through a cross section at $m + 1/2$ in a time interval $[0, T]$.

$$\mathcal{N} = \int_0^T dt \sum_{k \in BZ} \langle \Psi_1(k,t) | \hat{j}_{m+1/2}(t) | \Psi_1(k,t) \rangle$$

Pumped probability current and Berry curvature



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Here $\Psi_1(k,t) \approx |k\rangle \otimes |\tilde{u}_1(k,t)\rangle$

Pumped probability current and Berry curvature

We can write

$$
\begin{aligned}
\mathcal{N} &= \int_0^T dt \sum_{k\in BZ} \langle \tilde{u}_1(k,t)|\hat{j}_{m+1/2}(k,t)|\tilde{u}_1(k,t)\rangle \\
&= \frac{1}{N}\int_0^T dt \sum_{k\in BZ} \langle \tilde{u}_1(k,t)|\partial_k \hat{H}(k,t)|\tilde{u}_1(k,t)\rangle
\end{aligned}
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We insert

$$
|\tilde{u}_1(k,t)\rangle = e^{-i\int_0^t dt' E_1(k,t')}\left[|u_1(k,t)\rangle + i\frac{\langle u_2(k,t)|\partial_t|u_1(k,t)\rangle}{E_2(k,t)-E_1(k,t)}|u_2(k,t)\rangle\right]
$$

Pumped probability current and Berry curvature

$$\langle \tilde{u}_1(k,t)|\hat{j}_{m+1/2}(k,t)|\tilde{u}_1(k,t)\rangle = v_1(k,t) + i\frac{\langle u_1|\partial_k \hat{H}|u_2\rangle\langle u_2|\partial_t|u_1\rangle}{E_2 - E_1} + c.c$$

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When sumed over the Brillouin zone, the contribution $\sim v_1(k,t)$ will vanish.

Pumped probability current and Berry curvature

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When sumed over the Brillouin zone, the contribution $\sim v_1(k,t)$ will vanish.

Next, we use that

$$\langle u_1|\partial_k \hat{H}|u_2\rangle = (E_1 - E_2)\langle \partial_k u_1|u_2\rangle$$

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therefore

$$-\frac{\langle u_1|\partial_k \hat{H}|u_2\rangle\langle u_2|\partial_t|u_1\rangle}{E_2 - E_1} + c.c = -i\langle \partial_k u_1|u_2\rangle\langle u_2|\partial_t|u_1\rangle + c.c.$$

Pumped probability current and Berry curvature

Using the parallel transport gauge $\langle u_1|\partial_t|u_1\rangle = 0$, one can write

$$\begin{aligned}
-i\langle\partial_k u_1|u_2\rangle\langle u_2|\partial_t|u_1\rangle + c.c. &= -i\langle\partial_k u_1|\partial_t u_1\rangle + c.c \\
&= -i(\langle\partial_k u_1|\partial_t u_1\rangle - \langle\partial_t u_1|\partial_k u_1\rangle) \\
&= -i(\partial_k\langle u_1|\partial_t u_1\rangle) - \partial_t\langle u_1|\partial_k u_1\rangle)
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Finally, the number of pumped particles in a given driving cycle is

$$\mathcal{N} = \int_0^T dt \int_{BZ} \frac{dk}{2\pi}\Omega^{(1)}(k,t)$$

given by the integral of the Berry curvature.

Pumped probability current and Berry curvature

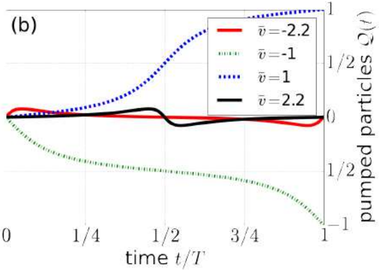

Figure : Number of pumped particles as a function of time.

Pumped probability current and Berry curvature

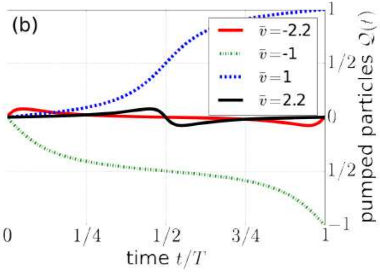

Figure : Number of pumped particles as a function of time.

Does it have to be an integer number ?

Overview

1) Model system
2) Particle current and group velocity
3) Quasi adiabatic time evolution
4) Pumped current and Berry curvature
5) Anomalous velocity of electrons

Anomalous velocity of electrons

Let us consider a crystal under the perturbation of a weak electric field $\mathbf{E}$. We represent the electric field through a uniform vector potential $\mathbf{A}(t)$ which is time dependent.

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Using minimal coupling theory, the Hamiltonian can be written

$$H(t) = \frac{[\hat{\mathbf{p}} + e\mathbf{A}]^2}{2m_e} + V(\mathbf{r})$$

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Because of the translation invariance, the solutions are Bloch wave functions.
The Hamiltonian that acts on the lattice periodic part of the Bloch wave functions can be written

$$H(\mathbf{k}, t) = H\left(\mathbf{k} + \frac{e}{\hbar}\mathbf{A}(t)\right)$$

Anomalous velocity of electrons

Since **A** preserves translation invariance, **k** is a good quantum number and is a constant of motion. Therefore

$$\frac{d}{dt}\mathbf{q} = \frac{d}{dt}\left(\mathbf{k} + \frac{e}{\hbar}\mathbf{A}(t)\right) = \frac{e}{\hbar}\frac{d}{dt}\mathbf{A}(t) = -\frac{e}{\hbar}\mathbf{E}$$

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One can define the average velocity in band n as a function of **q**:

$$\mathbf{v}^{(n)}(\mathbf{q}) = \langle u_n(\mathbf{k}, t)|\partial_{\mathbf{q}}\hat{H}|u_n(\mathbf{k}, t)\rangle$$

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Using

i) the results for the adiabatic evolution of $|u_n(\mathbf{k}, t)\rangle$

ii) that $\partial/\partial k_i = \partial/\partial q_i$ and $\partial/\partial t = -(e/\hbar)E_i\partial/\partial q_i$

Anomalous velocity of electrons

One can write the average velocity as

$$\mathbf{v}^{(n)}(\mathbf{q}) = \frac{\partial E_n(\mathbf{q})}{\hbar \partial \mathbf{q}} - \frac{e}{\hbar}\mathbf{E} \times \boldsymbol{\Omega}^{(n)}(\mathbf{q})$$

where $\Omega^{(n)}(\mathbf{q})$ is the Berry curvature of the nth band

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One can see that there is an *anomalous velocity* component

$$\frac{e}{\hbar}\mathbf{E} \times \boldsymbol{\Omega}^{(n)}(\mathbf{q})$$

which is *transverse* to the electric field.

Symmetry considerations

The velocity $\mathbf{v}^{(n)}(\mathbf{q})$ should obey certain symmetry constraints:

i) under time reversal, $\mathbf{v}^{(n)}$ and $\mathbf{q}$) change sign, while $\mathbf{E}$ is fixed

ii) under spatial inversion, $\mathbf{v}^{(n)}$, $\mathbf{q}$), $\mathbf{E}$ change sign

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This requires that

i) if the unperturbed system has time reversal symmetry then $\boldsymbol{\Omega}^{(n)}(-\mathbf{q}) = -\boldsymbol{\Omega}^{(n)}(\mathbf{q})$
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In crystals with simultaneous time-reversal and inversion symmetry the Berry curvature vanishes in the whole Brillouin zone.