Adiabatic vs Sudden Flux Insertion and Nonlinear Electric Conduction

Talk 2 by Masaki Oshikawa (ISSP, UTokyo)

Condensed Matter Physics
in All the Cities 2020
26 June 2020@Zoom

This presentation file is based on what was used in the actual talk at #CMPCity2020, but slightly revised and modified

Talk 1 (Last week, Thursday 18 June)

Applications of Adiabatic Flux Insertion to Quantum Many-Body Systems: A Pedagogical Introduction

M. O. and T. Senthil, PRL **96**, 060601 (2006)

Talk 2 (Today, Friday 26 June)

Adiabatic vs Sudden Flux Insertion and Nonlinear Electric Conduction

M. O. PRL **84**, 1535 (2000) / PRL **90**, 236401; **90** 109901 (E) (2003)
Haruki Watanabe and M.O., arXiv:2003.10390
Haruki Watanabe, Yankang Liu, and M. O., arXiv:2004.04561

Adiabatic Flux Insertion

(i) Increase Aharonov-Bohm flux Φ adiabatically from 0 to $\Phi_0 (=2\pi)$ $|\Psi_0\rangle \to |\Psi_0'\rangle$

Hamiltonian for the final state is different from the original one, but we can

(ii) eliminate the unit flux quantum by the large gauge transformation

$$U_x \mathcal{H}(\Phi = 2\pi) U_x{}^{-1} = \mathcal{H}(\Phi = 0)$$

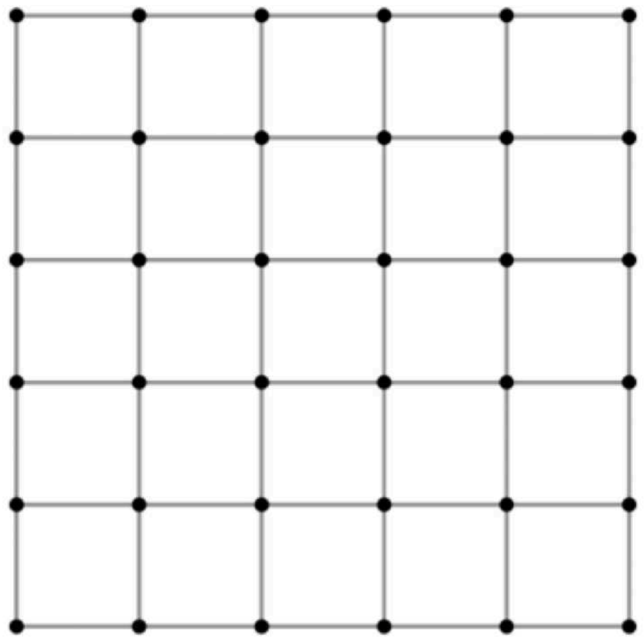
$$U_x = \exp\left(\frac{2\pi i}{L_x} \sum_{\vec{r}} x n_{\vec{r}} \right)$$

$$|\Psi_0\rangle \to |\Psi_0'\rangle \to U_x |\Psi_0'\rangle$$

Many Particles on Periodic Lattice

For example, consider a many-particle system on the square lattice of $L_x \times L_y$ with periodic boundary conditions

assume particle number conservation (U(1) symmetry)



assume that the system is gapped, and consider the adiabatic insertion of unit flux quantum through the "hole"

M. O. 2000

Translation Invariance

Translation invariance ⇒ Momentum Conservation

$$\vec{P} = -i\vec{\nabla}$$

Lattice model / periodic potential

discrete (lattice) translation: $T_x = e^{iP_x}$

Let us now consider the adiabatic flux insertion

$$A_x = \frac{\Phi_0 t}{T L_x}$$

Hamiltonian is always translation invariant

⇒ momentum is exactly conserved!

initial state: $P_x^{(0)}$ ⇒ final state: $P_x^{(0)}$

Which Momentum?

What is conserved exactly is the
"canonical momentum" which is NOT gauge-invariant!

$$\vec{P}_{\text{canonical}} = -i\vec{\nabla} \qquad\qquad \vec{P}_{\text{kinetic}} = -i\vec{\nabla} - \vec{A}$$

kinetic momentum = covariant derivative
(gauge invariant)

After the insertion of the unit flux quantum,
the system is equivalent to zero flux but in the different gauge!
We must eliminate the vector potential
by the large gauge transformation

Large Gauge Transformation

Initial Groundstate $|\Psi_0\rangle$

$$T_x|\Psi_0\rangle = e^{iP_x^{(0)}}|\Psi_0\rangle$$

groundstate of $\mathcal{H}(0)$

Final State $|\Psi_0'\rangle = \mathcal{F}_x|\Psi_0\rangle$

$$T_x|\Psi_0'\rangle = e^{iP_x^{(0)}}|\Psi_0'\rangle$$

groundstate of $\mathcal{H}(2\pi)$

Large gauge transformation

$|\tilde{\Psi}_0'\rangle \equiv U_x|\Psi_0'\rangle$ must be a groundstate of $\mathcal{H}(0)$

$$U_x = \exp\left(\frac{2\pi i}{L_x}\sum_{\vec{r}} x n_{\vec{r}}\right) \qquad {U_x}^{-1} T_x U_x = T_x \exp\left(\frac{2\pi i}{L_x}\sum_{\vec{r}} n_{\vec{r}}\right)$$

$$T_x|\tilde{\Psi}_0'\rangle = e^{i\left(P_x^{(0)} + \frac{2\pi}{L_x}\sum_{\vec{r}} n_{\vec{r}}\right)}|\tilde{\Psi}_0'\rangle$$

Momentum Shift

$$P_x^{(0)} \to P_x^{(0)} + \frac{2\pi}{L_x} \boxed{\sum_{\vec{r}} n_{\vec{r}}}$$

total number of particles (conserved)

We are usually interested in the thermodynamic limit for a fixed particle density (particle # / unit cell) ν

Suppose $\nu = \frac{p}{q}$ and choose L_y to be a coprime with q

$$\Delta P_x = \frac{2\pi}{L_x} L_x L_y \nu = 2\pi L_y \frac{p}{q}$$

Lattice momentum is defined modulo 2π

momentum shifted if $q \neq 1$ (fractional filling)

The final state is different from the initial ground state

⇒ **ground-state degeneracy!**

"Lieb-Schultz-Mattis Theorem"

General constraint on the spectrum of
quantum many-body Hamiltonian on a periodic lattice

Periodic (translation invariant) lattice ⇒ unit cell

U(1) symmetry ⇒ conserved particle number

ν : number of particle per unit cell (filling fraction)

$\nu = p/q \quad \Rightarrow$

"ingappability"

- system is gapless

OR

- gapped with q-fold degenerate ground states

~~gapped with unique ground state~~

History of the LSM Theorem

1961 **LSM** S=1/2 chain

1981 [**Haldane** "conjecture", dependence on 2S mod 2]

1986 **Affleck-Lieb** LSM theorem for general S chain

1997 **M.O.-Yamanaka-Affleck** general magnetization

1997 **Yamanaka-M.O.-Affleck** electrons/particles

2000 **M. O.** "flux insertion" argument for $d \geqq 2$

2004 **Hastings** rigorous proof

2006 **Nachtergale-Sims** really rigorous proof

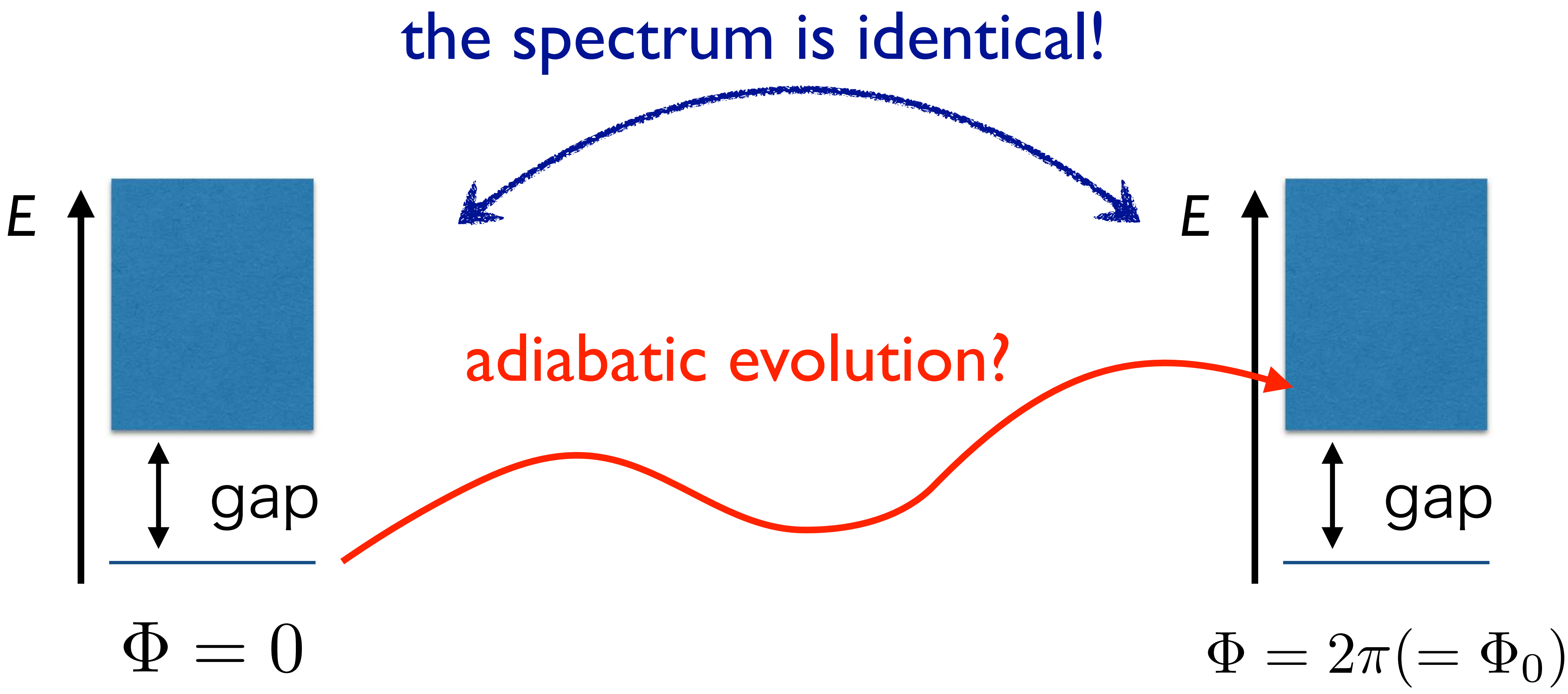
…

many recent extensions!

(non-symmorphic crystal symmetry

Parameswaran et al. 2013 etc.)

Gap Closing by AB Flux?



In principle, the ground state could evolve into an excited state, if there is a gap closing (level crossing with the "excited state") at some value of Φ

Insulator vs Conductor

Linear response theory: current induced by electric field

$$\vec{j}(\omega,\vec{q}) = \sigma(\omega,\vec{q})\vec{E}(\omega,\vec{q})$$

$$\sigma(\omega) \equiv \sigma(\omega,\vec{q}=0)$$

Drude weight

$$\sigma(\omega) = \frac{iD}{\pi}\frac{1}{\omega + i\delta} + \text{regular part}$$

$\delta \to +0$

$D=0$: insulator

$D>0$: conductor

(Kohn, 1963)

In a realistic system, the Drude peak is broadened ($\delta>0$), but in an ideal model we can identify delta-function Drude peak as a signature of ***"perfect conductor"***

Real-Time Formulation of *D*

$$j_x(t) \sim \int_{-\infty}^{t} \sigma(t-t')E_x(t')\,dt'$$

$$\lim_{t\to\infty} \sigma(t) = D$$

current induced by the electric field at *t*=0, that survives after an infinitely long time

Initial condition at *t*=0: ground state $|\Psi_0\rangle$

switch on an (infinitesimal) constant electric field for *t*>0

$$A_x = \mathcal{A}_x \frac{t}{T} \qquad E_x = \frac{\mathcal{A}_x}{T}$$

adiabatic limit $T \to \infty$

$$j_x(t) \sim D\frac{\mathcal{A}_x}{T}t$$

M. O. 2003

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Current vs Energy

On the other hand, the current operator is

V: volume

$$\hat{j}_x = \frac{1}{V}\frac{\partial \mathcal{H}}{\partial A_x}(A_x) = \frac{1}{V}\left(\frac{dA_x}{dt}\right)^{-1}\frac{\partial \mathcal{H}}{\partial t}$$

$$\boxed{j_x(t) \sim D\frac{\mathcal{A}_x}{T}t}$$

For an adiabatic flux insertion

$$\frac{1}{V}\Delta\mathcal{E}_0 = \frac{1}{V}\int_0^T \langle\frac{\partial \mathcal{H}}{\partial t}\rangle\, dt = \frac{\mathcal{A}_x}{T}\int_0^T j_x(t)\, dt \sim D\left(\frac{\mathcal{A}_x}{T}\right)^2\frac{T^2}{2}$$

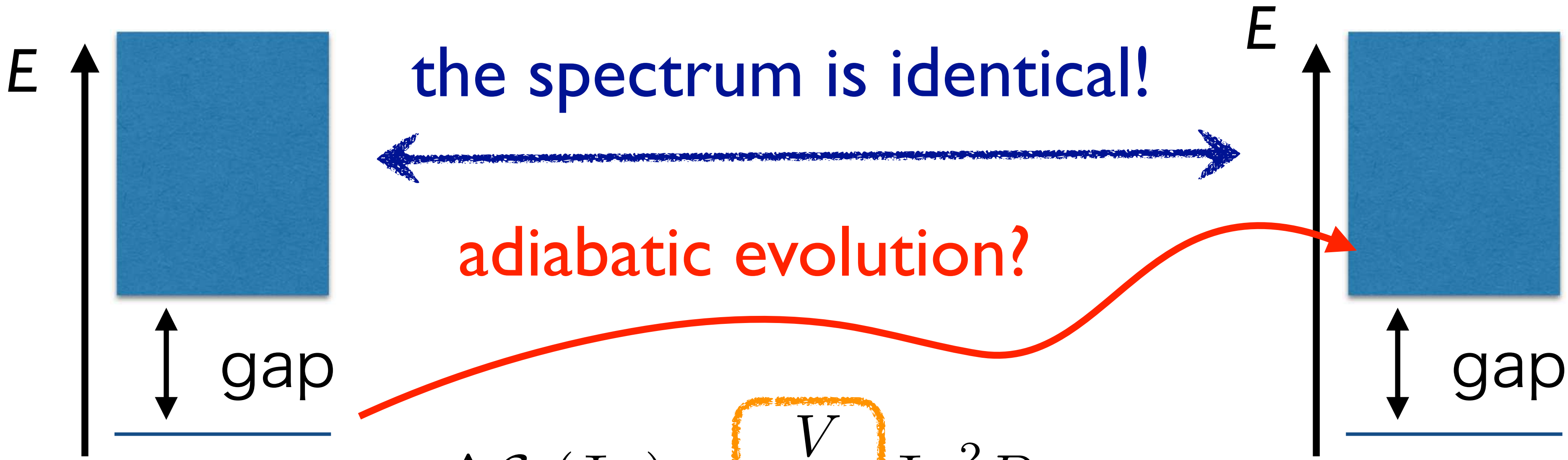
For the adiabatic insertion of unit flux quantum $\mathcal{A}_x = \frac{\Phi_0}{L_x}$

G. S. energy increase in the adiabatic flux insertion

$$\Delta\mathcal{E}_0(\Phi_0) = \frac{V}{2{L_x}^2}{\Phi_0}^2 D$$

M. O. 2003

Gap Protection in Insulators (d=2)



$\Phi = 0$

$$\Delta\mathcal{E}_0(\Phi_0) = \boxed{\frac{V}{2{L_x}^2}}{\Phi_0}^2 D$$

$O(L^{d-2})$

$\Phi = 2\pi(= \Phi_0)$

If this happens in d=2, energy gain ≧ gap ⇒ **D>0** !!

i.e. in an insulator, the groundstate must remain in the groundstate in the adiabatic flux insertion ⇒ LSM

Kohn Formula

$$\Delta\mathcal{E}_0(\Phi_0) = \frac{V}{2{L_x}^2}{\Phi_0}^2 D$$

$$\mathcal{A}_x = \frac{\Phi_0}{L_x} \to 0$$

$$D = \frac{1}{V}\ \frac{\partial^2\mathcal{E}_0}{\partial{\mathcal{A}_x}^2}(\mathcal{A}_x)\Big|_{\mathcal{A}_x=0}$$

Kohn's formula for the Drude weight

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

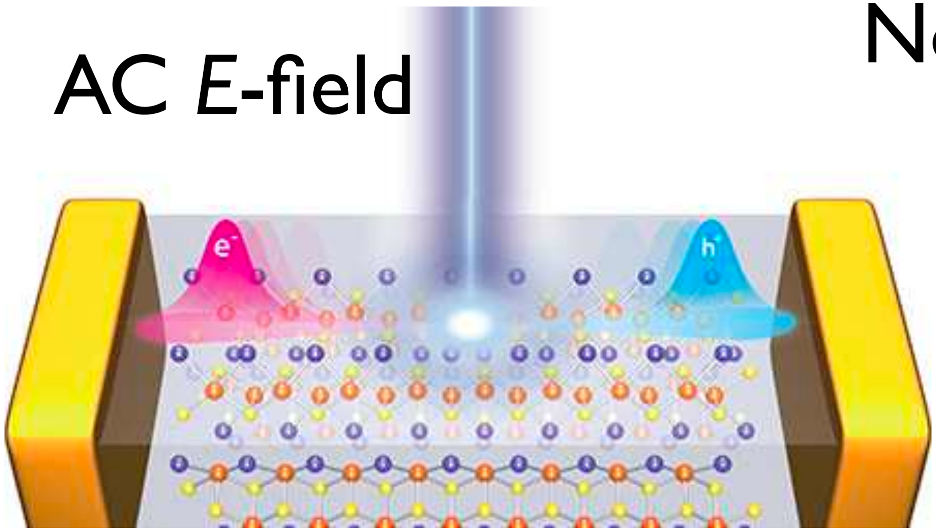
Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by

Non-Linear Conductivities

AC E-field



DC current

Non-linear electric conduction: topic of current interest

e.g. "shift current"

application to photovoltaics

n-th order conductivity

$$j_x(t) \sim \sum_{n=1}^{\infty} \frac{1}{n!} \int_{-\infty}^{t} \cdots \int_{-\infty}^{t} \int_{-\infty}^{t} \sigma^{(n)}(t-t_1, t-t_2, \ldots, t-t_n)$$

$$E_x(t_1) E_x(t_2) \ldots E_x(t_n) \, dt_1 dt_2 \ldots dt_n$$

Nonlinear Drude weights

$$\lim_{\Delta t_1, \Delta t_2, \ldots, \Delta t_n \to \infty} \sigma^{(n)}(\Delta t_1, \Delta t_2, \ldots, \Delta t_n) = D^{(n)}$$

Non-Linear "Kohn Formula"

Consider the same adiabatic flux insertion
and include the non-linear Drude weights

$$A_x = \mathcal{A}_x \frac{t}{T} \qquad\qquad j_x^{(n)}(t) \sim \frac{1}{n!} D^{(n)} \left(\frac{\mathcal{A}_x}{T} \right)^n t^n$$

$$\begin{aligned}\frac{1}{V} \Delta \mathcal{E}_0^{(n+1)} &= \frac{1}{V} \int_0^T \frac{\partial \mathcal{H}}{\partial t}\, dt = \frac{\mathcal{A}_x}{T} \int_0^T j_x^{(n)}(t)\, dt \\ &\sim \frac{1}{n!} D^{(n)} \left(\frac{\mathcal{A}_x}{T} \right)^{n+1} \frac{T^{n+1}}{n+1} = \frac{1}{(n+1)!} D^{(n)} {\mathcal{A}_x}^{n+1}\end{aligned}$$

$$\boxed{D^{(n)} = \frac{1}{V} \frac{\partial^{n+1} \mathcal{E}_0}{\partial {A_x}^{n+1}} (\mathcal{A}_x) \Big|_{\mathcal{A}_x = 0}}$$

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Sudden Flux Insertion

$$A_x = \mathcal{A}_x \frac{t}{T} \qquad E_x = \frac{\mathcal{A}_x}{T}$$

$T \to 0$: sudden insertion
delta-function electric field pulse

In this limit, quantum state (wavefunction) does not change

but again we are in a different gauge, so need to apply the large gauge transformation to go back to the original gauge

$$|\Psi_0\rangle \to |\Psi_0\rangle \to U_x|\Psi_0\rangle$$

Energy Gain in Sudden Flux Insertion

$$\boxed{\frac{1}{V}\Delta\mathcal{E}} = \frac{1}{V}\int_0^T \langle\frac{\partial\mathcal{H}}{\partial t}\rangle\, dt = \frac{\mathcal{A}_x}{T}\int_0^T j_x(t)\, dt$$

T→0

$$\sim \frac{\sigma^{(n)}(0,0,\ldots,0)}{2^n}\frac{1}{n+1}\left(\frac{\mathcal{A}_x}{T}\right)^n$$

$$j_x(t) \sim \sum_{n=1}^{\infty}\frac{1}{n!}\int_0^t \cdots \int_0^t \sigma^{(n)}(t-t_1,\ldots,t-t_n)\left(\frac{\mathcal{A}_x}{T}\right)^n dt_1 dt_2\ldots dt_n$$

$$\sim \frac{\sigma^{(n)}(0,0,\ldots,0)}{2^n}\left(\frac{\mathcal{A}_x}{T}\right)^n t^n$$

$$\frac{1}{V}\left(\langle\Psi_0|{U_x}^{\dagger}\mathcal{H}(0)U_x|\Psi_0\rangle - \langle\Psi_0|\mathcal{H}(0)|\Psi_0\rangle\right)$$

$$= \frac{1}{V}\langle\Psi_0|\left[\mathcal{H}(\mathcal{A}_x = \frac{\Phi_0}{L_x}) - \mathcal{H}(0)\right]|\Psi_0\rangle$$

cf.) LSM variational energy

Non-linear *f*-Sum Rules

Comparing both sides, we obtain the identity

instantaneous response in real-time

$$\frac{\sigma^{(n)}(0,0,\ldots,0)}{2^n} = \langle\Psi_0|\left.\frac{\partial^{n+1}\mathcal{H}(\mathcal{A}_x)}{\partial\mathcal{A}_x{}^{n+1}}\right|_{\mathcal{A}_x=0}|\Psi_0\rangle$$

$$= \int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega_2}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{d\omega_n}{2\pi}\sigma^{(n)}(\omega_1,\omega_2,\ldots,\omega_n)$$

[frequency space representation]

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cf.) Shimizu 2010, Shimizu-Yuge 2011

Example: Tight-Binding Model

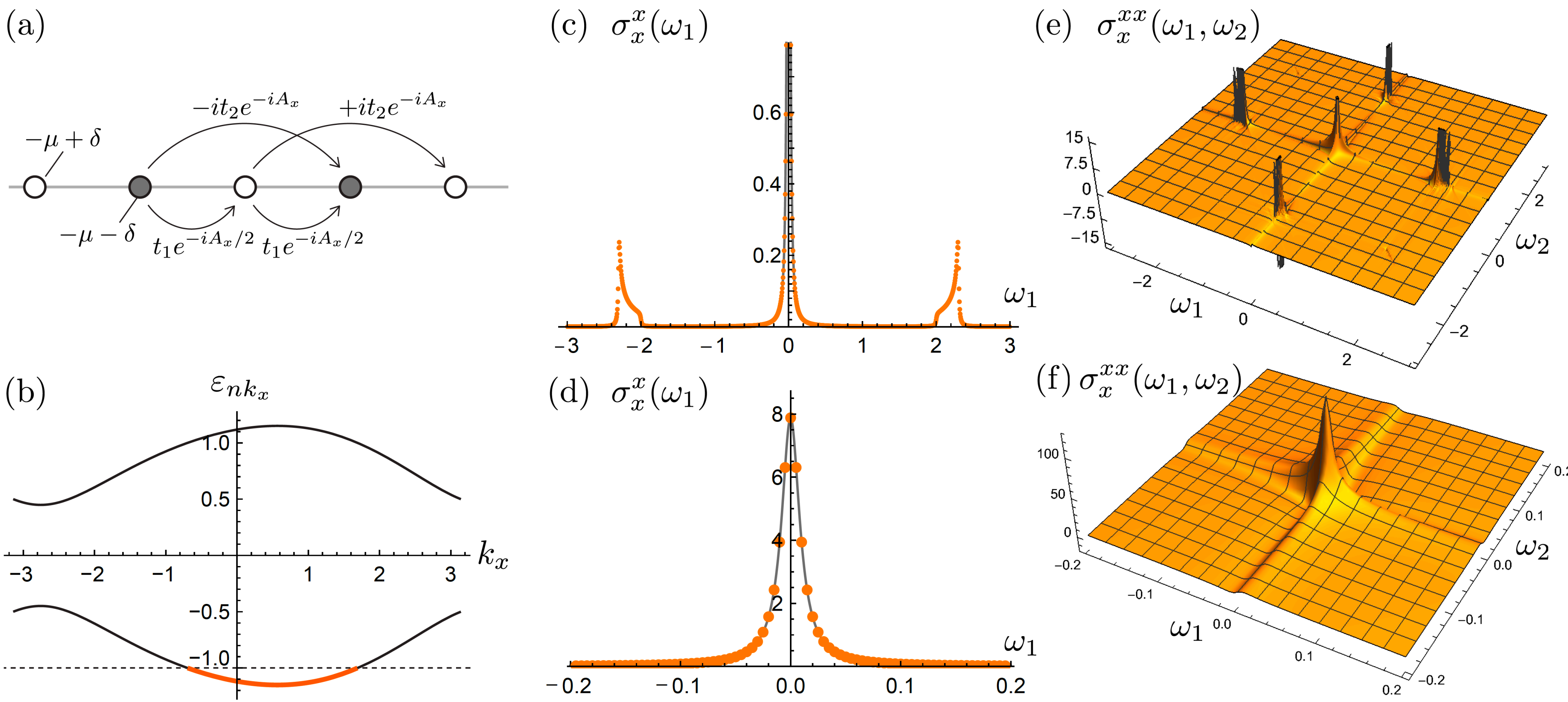

FIG. 1. The linear and the second-order optical conductivities in the tight-binding model in Eq. (74). (a) The real-space illustration of the model. (b) The band structure ε_{nk_x} as a function of k_x. The orange part is occupied in the ground state. (c) $\sigma_x^x(\omega_1)$ as a function of $\omega_1 \in (-3,3)$. The gray curve is the fit by Eq. (75). (d) The zoom up of (c) for $\omega_1 \in (-0.2,0.2)$. (e) $\sigma_x^{xx}(\omega_1,\omega_2)$ as a function of $\omega_1,\omega_2 \in (-3,3)$. (f) The zoom up of (e).

Numerical Check

TABLE I. Numerical results for the tight-binding model in Eq. (74). See the main text for the definitions of these quantities in the actual calculation.

Linear response $\sigma_x^x(\omega_1)$				Second-order response $\sigma_x^{xx}(\omega_1,\omega_2)$			
Drude weight		f-sum		Drude weight		f-sum	
$\mathcal{D}_x^x$	$\frac{1}{L_x}\frac{\partial^2\mathcal{E}_0(A_x)}{\partial A_x^2}$	$\int \frac{d\omega_1}{2\pi}\sigma_x^x(\omega_1)$	$\frac{1}{2L_x}\langle\frac{\partial^2\hat{H}(A_x)}{\partial A_x^2}\rangle_0$	$\mathcal{D}_x^{xx}$	$\frac{1}{L_x}\frac{\partial^3\mathcal{E}_0(A_x)}{\partial A_x^3}$	$\int\int \frac{d\omega_1 d\omega_2}{(2\pi)^2}\sigma_x^{xx}(\omega_1,\omega_2)$	$\frac{1}{4L_x}\langle\frac{\partial^3\hat{H}(A_x)}{\partial A_x^3}\rangle_0$
0.0788238	0.0788231	0.0487034	0.0487345	0.0122513	0.0122554	0.00594065	0.00596566

Summary

Two general formulas for non-linear conductivity

***f*-sum rules** (instantaneous response = ω-integral)

$$\frac{\sigma^{(n)}(0,0,\ldots,0)}{2^n} = \langle \Psi_0 | \left. \frac{\partial^{n+1}\mathcal{H}(\mathcal{A}_x)}{\partial {\mathcal{A}_x}^{n+1}} \right|_{\mathcal{A}_x=0} | \Psi_0 \rangle$$

energy gain by ***sudden*** flux insertion

"Kohn formulas" for non-linear Drude weights

(long-time response = 1/ω pole)

$$D^{(n)} = \frac{1}{V} \left. \frac{\partial^{n+1}\mathcal{E}_0}{\partial {\mathcal{A}_x}^{n+1}}(\mathcal{A}_x) \right|_{\mathcal{A}_x=0}$$

energy gain by ***adiabatic*** flux insertion

more general results are given in arXiv:2003.10390 & arXiv:2004.04561