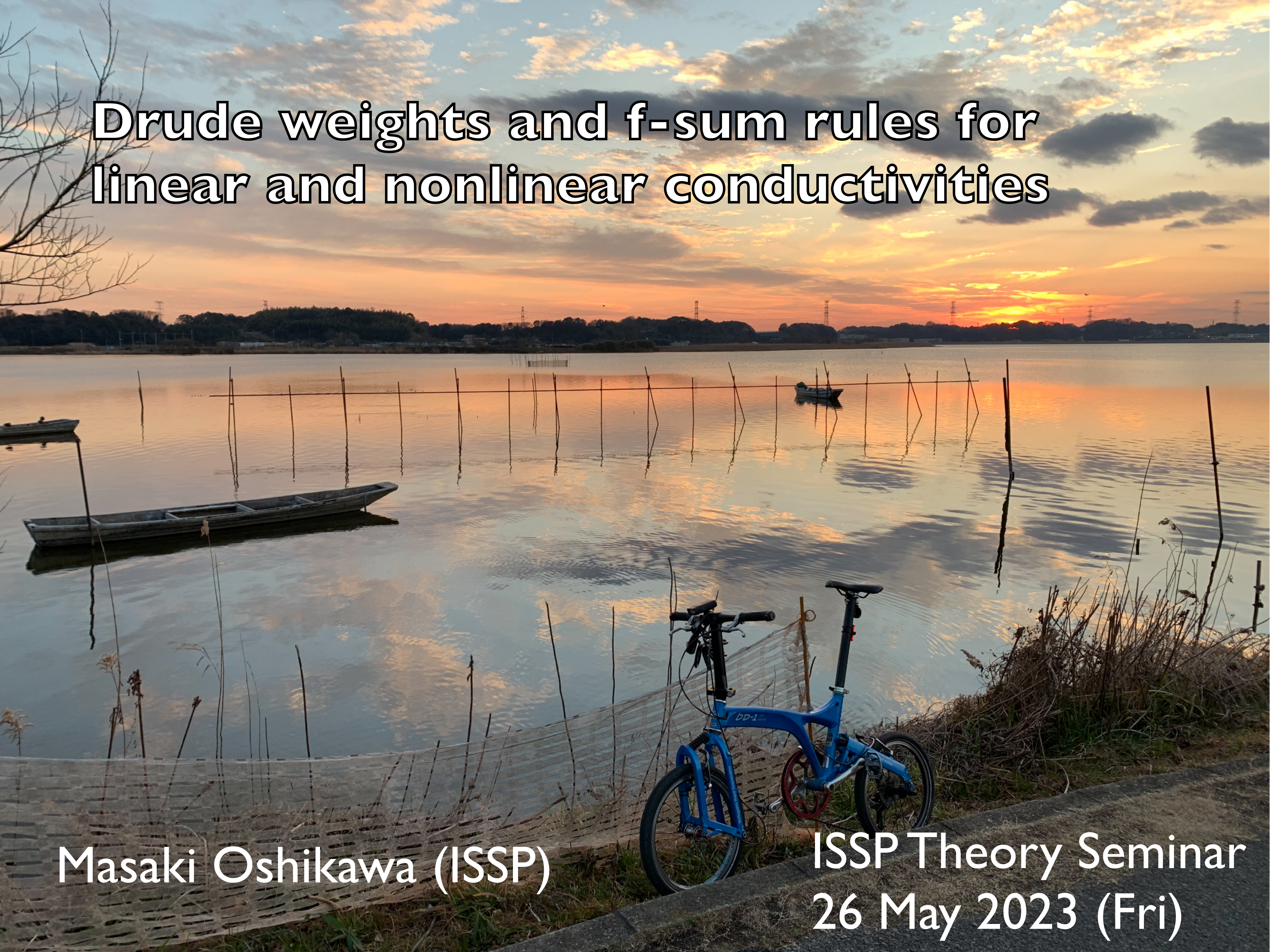


Drude weights and f-sum rules for linear and nonlinear conductivities

Masaki Oshikawa (ISSP)

ISSP Theory Seminar
26 May 2023 (Fri)

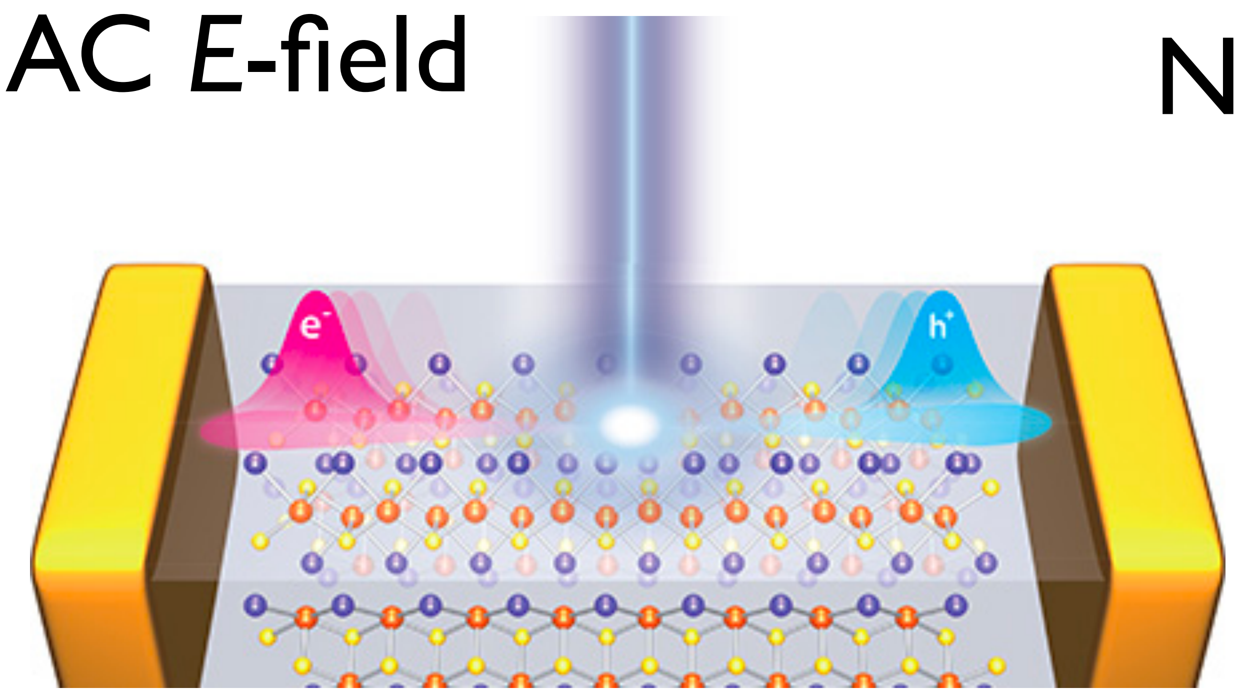
Non-Linear Conductivities

n-th order conductivities

$$j \sim \sigma^{(1)} E + \sigma^{(2)} EE + \sigma^{(3)} EEE + \dots$$

renewed interest thanks to developments in laser technology, theory, ……

AC *E*-field



DC current

Non-linear electric conduction: topic of current interest

e.g. "shift current"

$$j \propto E^2$$

application to photovoltaics

This Talk

General constraints on nonlinear conductivities

- nonlinear *f*-sum rules
- nonlinear Kohn formula for Drude weights

in a unified formulation

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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

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

$\delta \to +0$

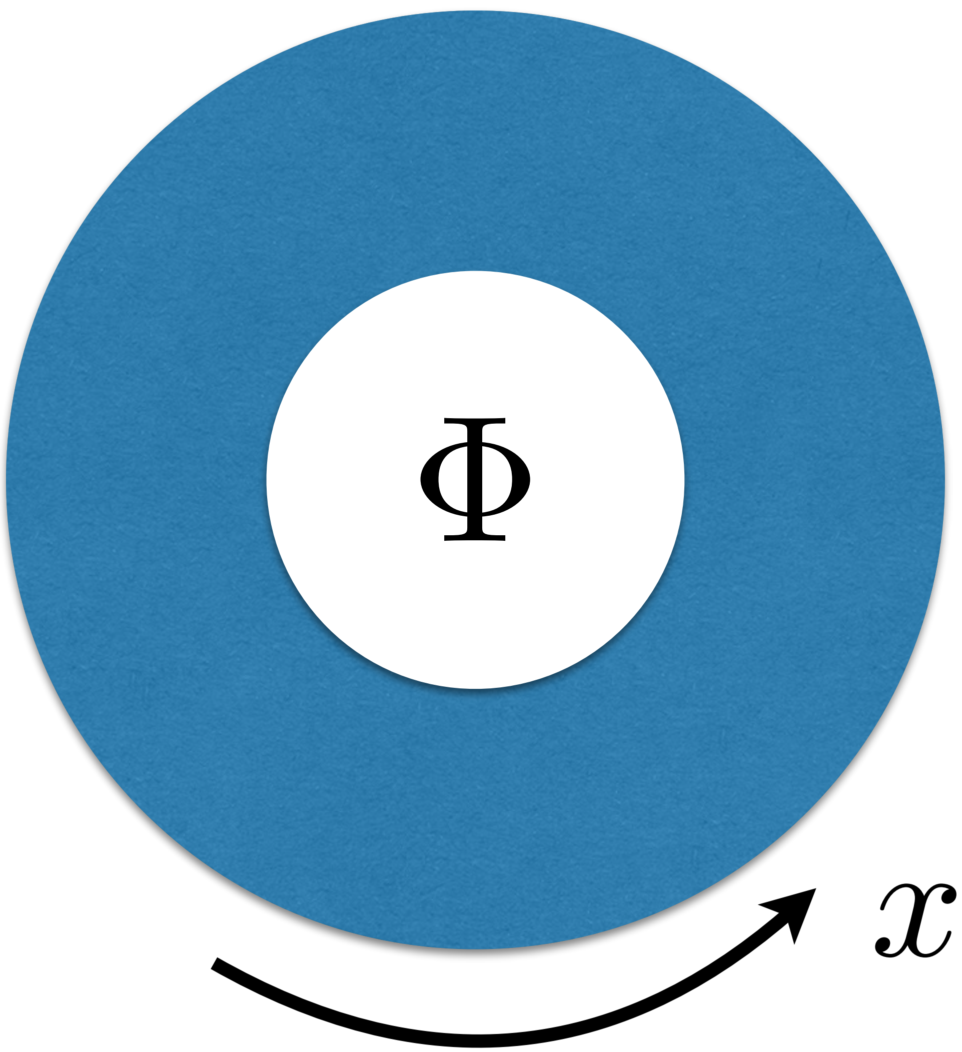
D=0 : insulator

D>0 : conductor

(Kohn, 1964)

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"***

Aharonov-Bohm Effect



particles do not touch
the magnetic field directly
⇒ no effect within classical mech

But quantum interference is still affected ⇒

Aharonov-Bohm effect

Quantum system defined on the annulus does depend on the flux, except when the Aharonov-Bohm phase is

$$\Phi = 2\pi \times \text{integer}$$

Unit Flux Quantum

I have implicitly chosen the units so that

$$\hbar = 1 \qquad\qquad e = 1$$

Covariant derivative ⇔ kinetic momentum

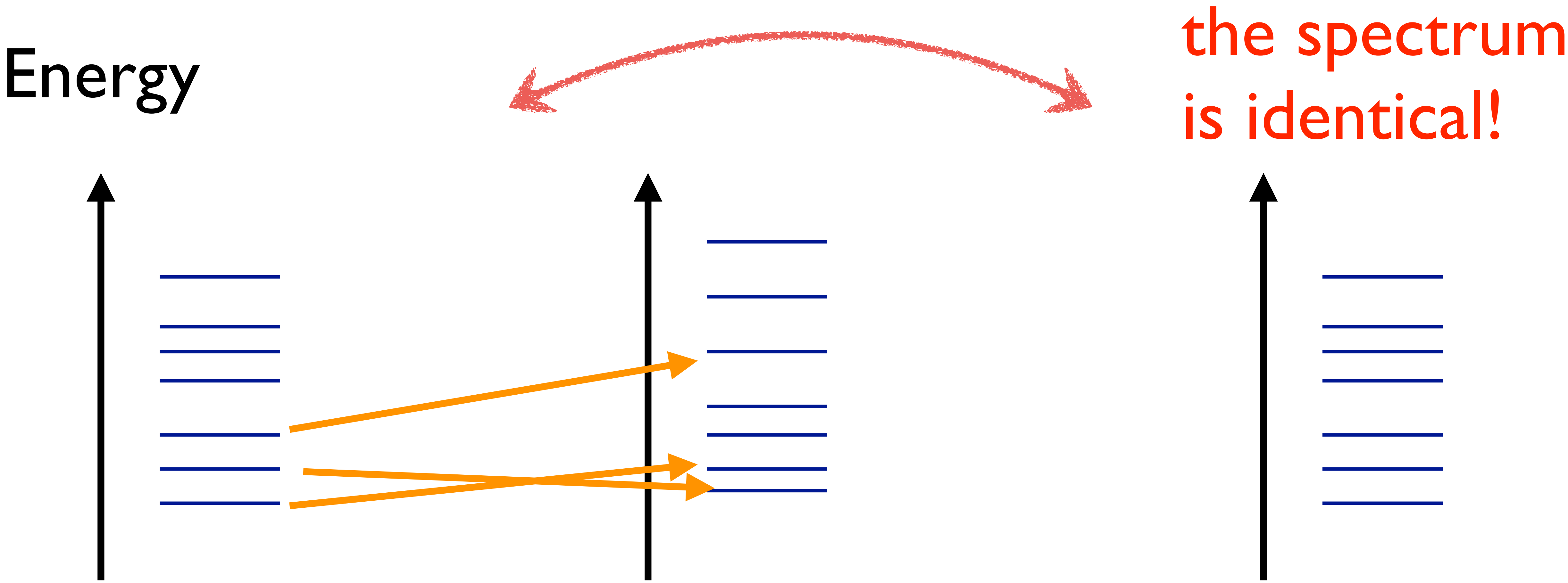
$$\left(-i\hbar\vec{\nabla} - e\vec{A}(\vec{r})\right)\psi(\vec{r})$$

$$\exp\left(i\frac{e}{\hbar}\oint_{\partial S}\vec{A}(\vec{r})\cdot d\vec{r}\right) = \exp\left[2\pi i\frac{\Phi(S)}{\Phi_0}\right]$$

$$\Phi_0 = \frac{h}{e} = 4.136 \times 10^{-15}\ \mathrm{Wb}$$

(twice the "unit flux quantum" commonly used in superconductivity literature)

Spectrum of the Hamiltonian



$\Phi = 0$

generally depends on Φ (AB effect)

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

Nevertheless $\mathcal{H}(\Phi = 2\pi) \neq \mathcal{H}(\Phi = 0)$

Large Gauge Transformation

If the Aharonov-Bohm flux is an integral multiple of the unit flux quantum it can be eliminated by a topologically nontrivial ("large") gauge transformation

$$\psi(\vec{r}) \to \psi(\vec{r})e^{i\theta(\vec{r})} \qquad \theta(\vec{r}) = 2\pi\frac{x}{L_x}$$

phase is multivalued but wavefunction is unique

For a many-body Hamiltonian on a lattice

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

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

Adiabatic Unit Flux Quantum Insertion

(i) Increase Aharonov-Bohm flux Φ adiabatically from 0 to Φ_0(=2π)

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

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

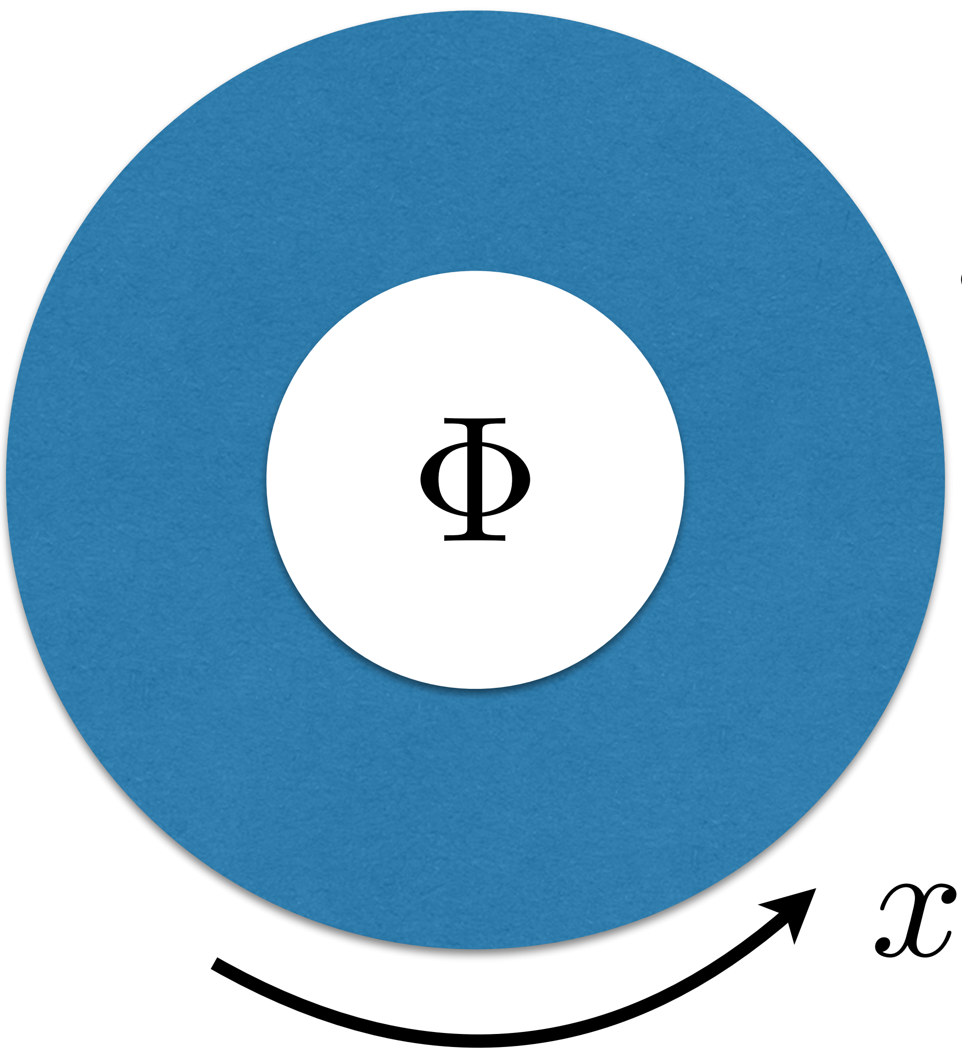
$$U_x \mathcal{H}(\Phi = 2\pi) {U_x}^{-1} = \mathcal{H}(\Phi = 0)$$

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

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

Final state may be different from the original ground state

Time-Dependent Flux and Electric Field



particles do not touch the magnetic field directly ⇒

static flux has no effect within classical mech

vector potential $A_x = \dfrac{\Phi}{L_x}$

However, a time-dependent flux does induce an electric field, either in a classical or quantum system

Time-dependent flux ⇒ induced electric field

$$\frac{1}{L_x}\frac{d\Phi}{dt} = \frac{dA_x}{dt} = E_x$$

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 $T \to \infty$

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

M. O. 2003
Watanabe-M.O. 2020

Current vs Energy

On the other hand, the current operator is

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

V: volume

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

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

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

Nonlinear Drude Weights

Nonlinear conductivities (real-time form)

$$j_x(t) \sim \sum_{n=1}^{\infty} \frac{1}{n!} \int_{-\infty}^{t} \cdots \int_{-\infty}^{t} \int_{-\infty}^{t} \sigma^{(n)}(t-t_1, t-t_2, \ldots, t-t_n)$$
$$E_x(t_1) E_x(t_2) \ldots E_x(t_n) \, dt_1 dt_2 \ldots dt_n$$

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

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

$$\frac{1}{V}\Delta\mathcal{E}_0^{(n+1)} = \frac{1}{V}\int_0^T \frac{\partial \mathcal{H}}{\partial t}\, dt = \frac{\mathcal{A}_x}{T}\int_0^T j_x^{(n)}(t)\, dt$$

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

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

Watanabe-M.O. 2020
Watanabe-Liu-M.O. 2020

Sudden Unit Flux Quantum 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

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

$T \to 0$

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

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

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

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

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

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]

Watanabe-M.O. / Watanabe-Liu-M.O. 2020
cf.) Shimizu 2010, Shimizu-Yuge 2011

(Unexpected) Symmetries

$$\mathcal{D}_x^{yz} = \mathcal{D}_y^{zx} = \mathcal{D}_z^{xy} = \frac{\partial^3 \mathcal{E}(\vec{A})}{\partial A_x \partial A_y \partial A_z}\Big|_{\vec{A}=\vec{0}}.$$

$$\int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega_2}{2\pi} \sigma_x^{xy}(\omega_1, \omega_2)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega_2}{2\pi} \sigma_y^{xx}(\omega_1, \omega_2) = \frac{1}{4}\left\langle \frac{\partial^3 \hat{H}(\vec{A})}{\partial A_x^2 \partial A_y}\Big|_{\vec{A}=\vec{0}} \right\rangle_0$$

hold without any symmetry of the system!

Watanabe-M.O. 2020

Direct "Kubo Theory" Calculation

$$\hat{H}(t, \vec{A}(t)) = \sum_{N=0}^{\infty} \hat{H}_N(t), \qquad \hat{\rho}(t) = \sum_{N=0}^{\infty} \hat{\rho}_N(t).$$

$$\partial_t \hat{\rho}_N(t) = \sum_{M=0}^{N} (-i)[\hat{H}_{N-M}(t), \hat{\rho}_M(t)].$$

$$\hat{\tilde{\rho}}_1(t) = \int_0^t dt' (-i)[\hat{\tilde{H}}_1(t'), \hat{\rho}_0],$$

$$\hat{\tilde{\rho}}_2(t) = \int_0^t dt' (-i)[\hat{\tilde{H}}_2(t'), \hat{\rho}_0] + \int_0^t dt' \int_0^{t'} dt'' (-i)^2 [\hat{\tilde{H}}_1(t'), [\hat{\tilde{H}}_1(t''), \hat{\rho}_0]],$$

Explicit Proof for 2nd Kohn formula

$$\sum_n \rho_n \frac{\partial^3 \mathcal{E}_n(\vec{A})}{\partial A_i \partial A_{i_1} \partial A_{i_2}}\Big|_{\vec{A}=\vec{0}}$$

$$= \sum_n \rho_n \frac{\partial^2}{\partial A_{i_1}\partial A_{i_2}} \Big\langle n(\vec{A}) \Big| \frac{\partial \hat{H}(\vec{A})}{\partial A_i} \Big| n(\vec{A}) \Big\rangle \Big|_{\vec{A}=\vec{0}}$$

$$= \mathcal{S}_{i_1 i_2} \sum_n \rho_n \big(\langle n | \hat{H}_{i i_1 i_2} | n \rangle + 2 \langle n_{i_1} | \hat{H}_i | n_{i_2} \rangle \big) + \mathcal{S}_{i_1 i_2} \sum_n \rho_n \big(2 \langle n | \hat{H}_{i i_1} | n_{i_2} \rangle + \langle n | \hat{H}_i | n_{i_1 i_2} \rangle \big) + \text{c.c.}$$

$$= \mathcal{S}_{i_1 i_2} \sum_n \rho_n \big(\langle n | \hat{H}_{i i_1 i_2} | n \rangle + 2 \langle n_{i_1} | \hat{Q}_n \delta_n \hat{H}_i \hat{Q}_n | n_{i_2} \rangle \big) + \mathcal{S}_{i_1 i_2} \sum_n \rho_n \big(2 \langle n | \hat{H}_{i i_1} \hat{Q}_n | n_{i_2} \rangle + \langle n | \hat{H}_i \hat{Q}_n | n_{i_1 i_2} \rangle \big) + \text{c.c.}$$

$$+ 2\mathcal{S}_{i_1 i_2} \sum_n \rho_n \langle n_{i_1} | \hat{Q}_n \hat{H}_i | n \rangle \langle n | n_{i_2} \rangle + \text{c.c.}$$

$$= \mathcal{S}_{i i_1 i_2} \sum_n \rho_n \Big[\langle n | \hat{H}_{i i_1 i_2} | n \rangle - 3 \langle n | \hat{H}_i \frac{\hat{Q}_n}{\hat{H}_0 - \mathcal{E}_n} \hat{H}_{i_1 i_2} | n \rangle + \text{c.c.} + 6 \langle n | \hat{H}_{i_1} \frac{\hat{Q}_n}{\hat{H}_0 - \mathcal{E}_n} \delta_n \hat{H}_i \frac{\hat{Q}_n}{\hat{H}_0 - \mathcal{E}_n} \hat{H}_{i_2} | n \rangle \Big]$$

$$= V \phi_i^{i_1 i_2}(\omega_1 = 0, \omega_2 = 0) = V \mathcal{D}_i^{i_1 i_2}.$$

Similar explicit proof for up to 3rd order
Kohn formula & *f*-sum rule Watanabe-Liu-M.O. 2020

Example: Tight-Binding Model

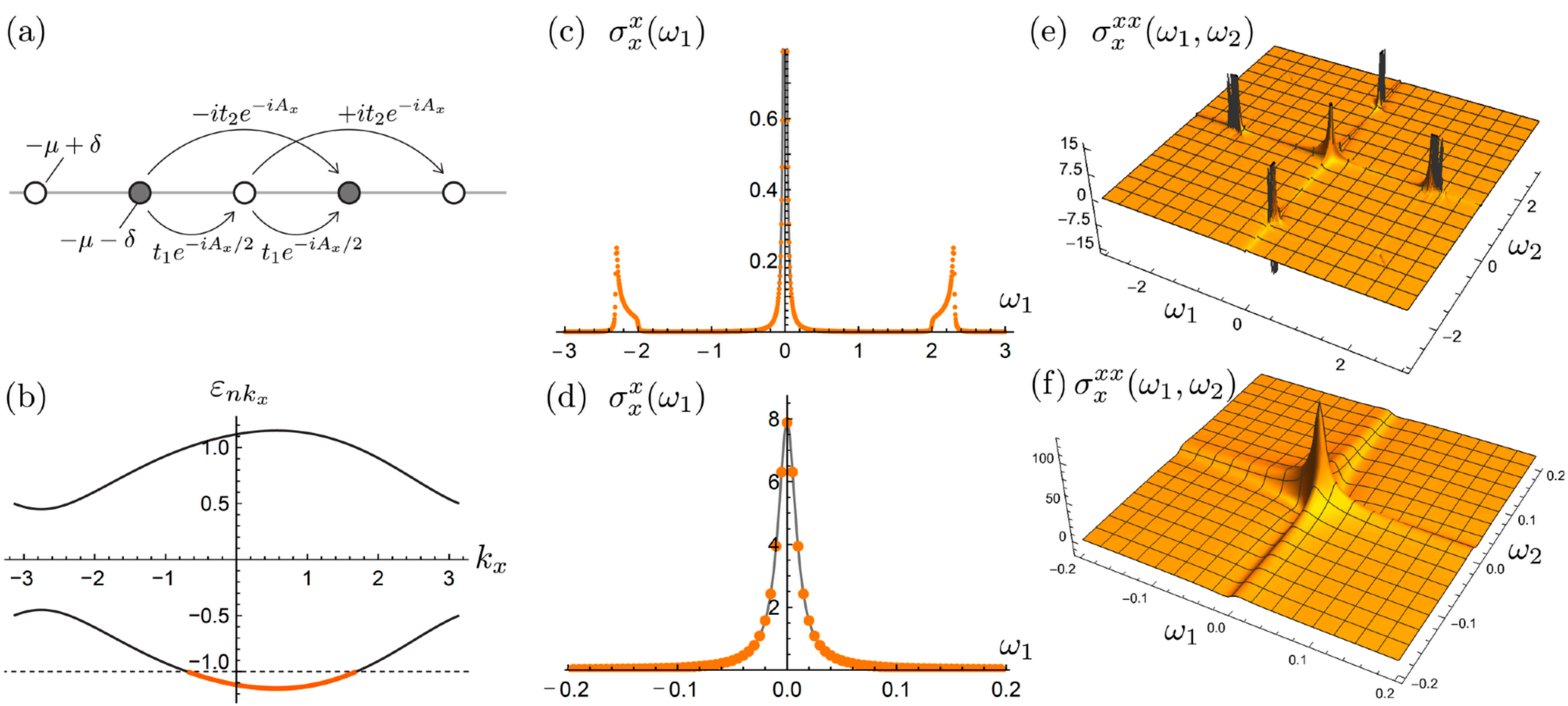


FIG. 1. The linear and the second-order optical conductivities in the tight-binding model in Eq. (74). (a) The real-space illustration of the model. (b) The band structure ε_{nk_x} as a function of k_x. The orange part is occupied in the ground state. (c) $\sigma_x^x(\omega_1)$ as a function of $\omega_1 \in (-3,3)$. 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

S=1/2 XXZ Chain

$$\hat{H}(A_x) = -J \sum_{x=1}^{L_x} \left(\frac{1}{2} \hat{s}^{+}_{x+1} e^{-iA_x} \hat{s}^{-}_{x} + \text{h.c.} + \Delta \hat{s}^{z}_{x+1} \hat{s}^{z}_{x} \right).$$

can be mapped to spinless fermion with
density-density **interaction**

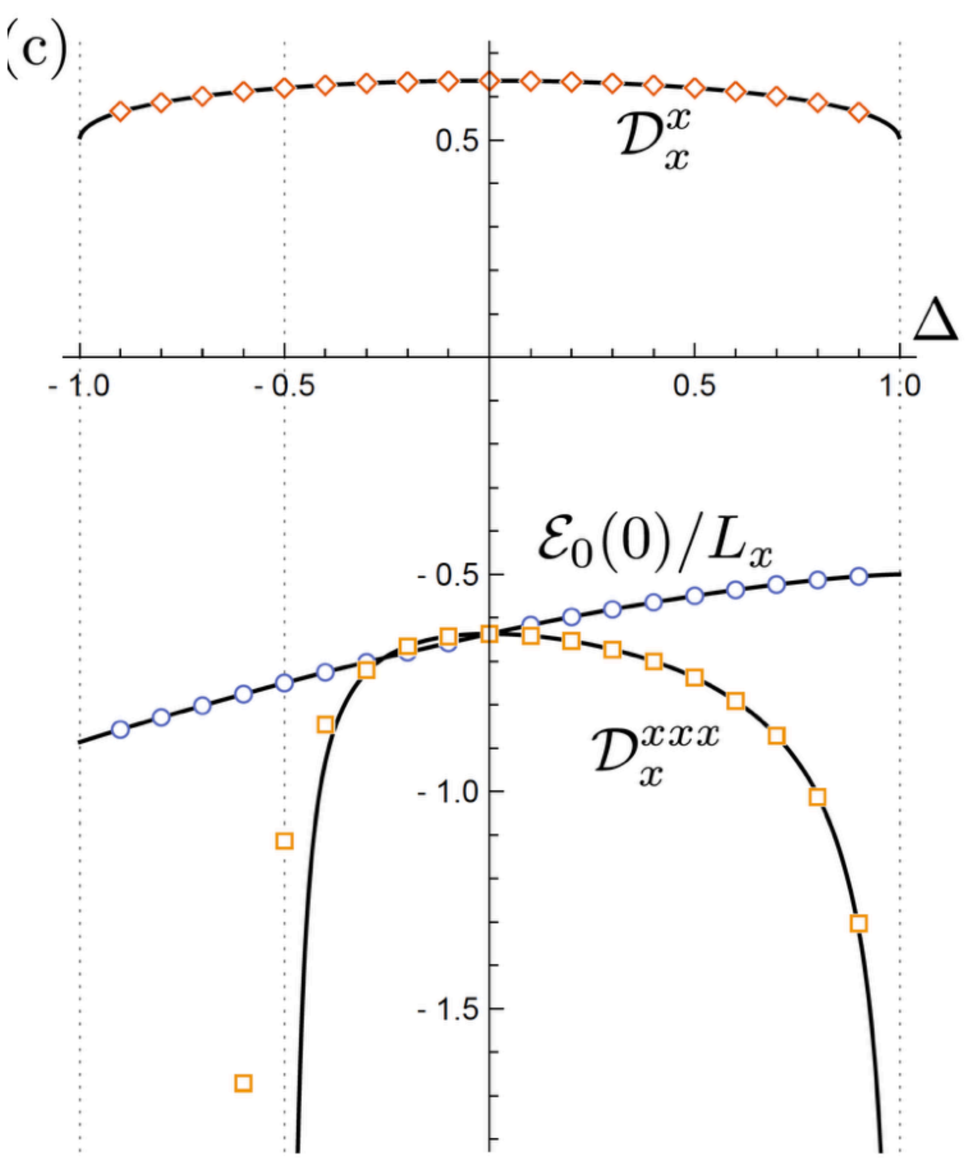
exactly solvable by Bethe Ansatz technique;
effective field theory (Tomonaga-Luttinger Liquid)

Ground-state energy density as a function of the flux

$$\frac{\mathcal{E}_{0,L_x}(A_x)}{L_x} = \frac{\mathcal{E}_{0,L_x}(0)}{L_x} + \frac{\mathcal{D}^{x}_{x,L_x} A_x^2}{2} + \frac{\mathcal{D}^{xxx}_{x,L_x} A_x^4}{24} + O(A_x^6).$$

Exact 3rd-order Drude Weight

$$\mathcal{D}_x^{xxx} = -\frac{J\sin\gamma}{16\gamma(\pi-\gamma)}\left(\frac{\Gamma\left(\frac{3\pi}{2\gamma}\right)\Gamma\left(\frac{\pi-\gamma}{2\gamma}\right)^3}{\Gamma\left(\frac{3(\pi-\gamma)}{2\gamma}\right)\Gamma\left(\frac{\pi}{2\gamma}\right)^3}+\frac{3\pi\tan\left(\frac{\pi^2}{2\gamma}\right)}{\pi-\gamma}\right)$$



$$\Delta = -\cos\gamma$$

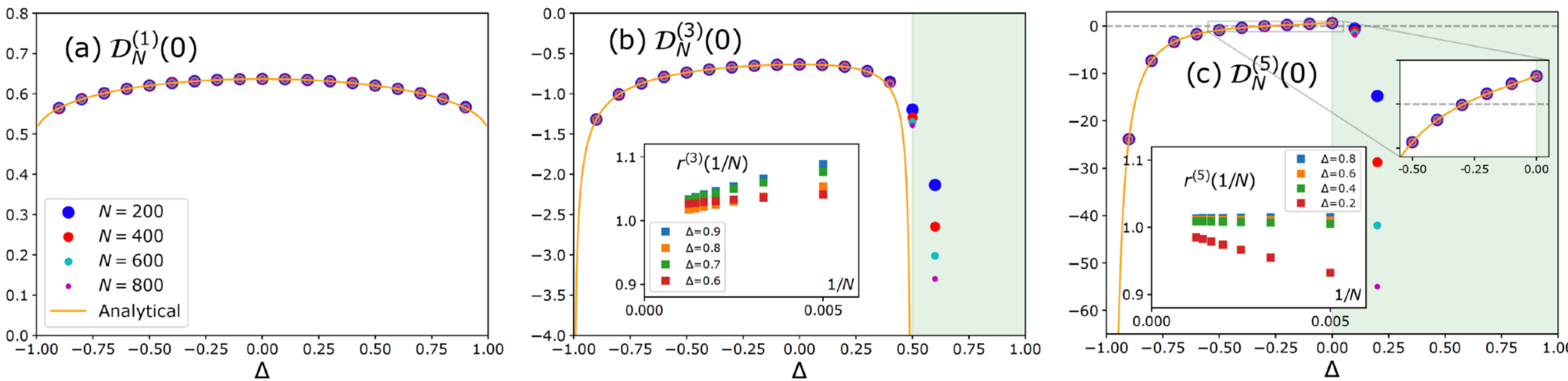
M.O.-Watanabe 2020
based on Lukyanov 1998

Good agreement with numerics

Divergent for Δ<-1/2 ?!

Recent Extension

Tanikawa-Takasan-Katsura 2021



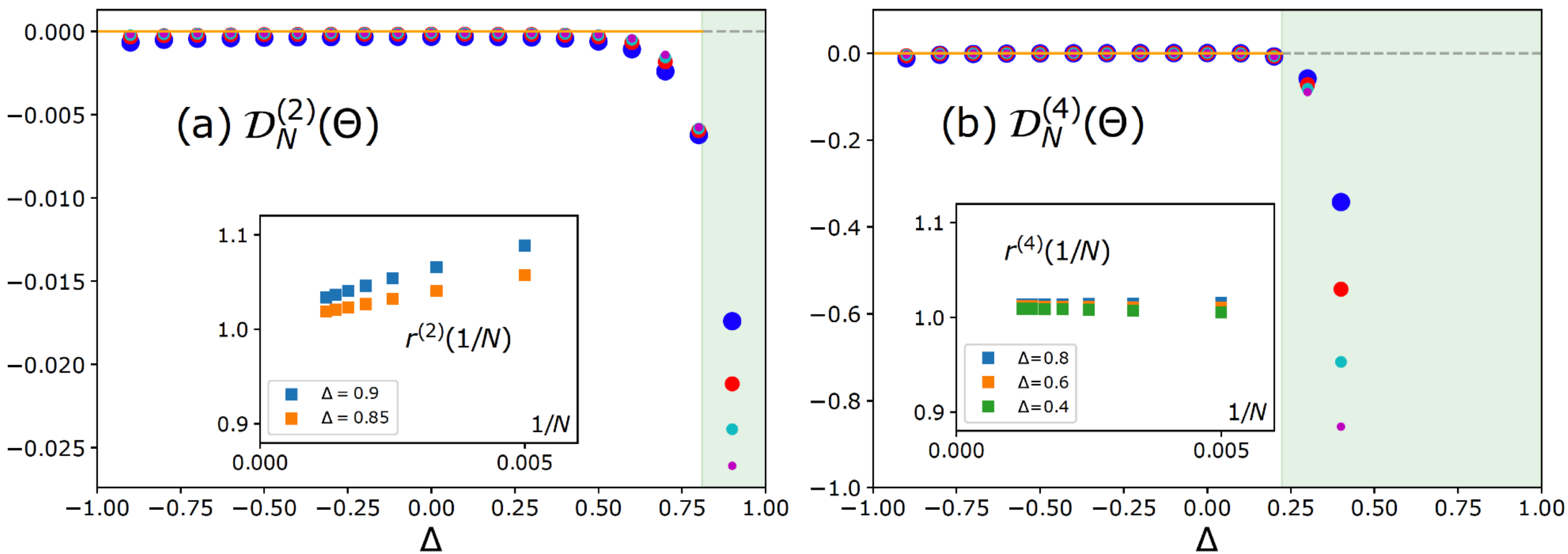
(sign of Δ is reversed in their paper)

$$\mathcal{D}^{(5)} = \frac{3J\sin\gamma}{32\pi\gamma(\pi-\gamma)}\left[\frac{\Gamma\left(\frac{5\pi}{2\gamma}\right)\Gamma\left(\frac{\pi-\gamma}{2\gamma}\right)^5}{\Gamma\left(\frac{5(\pi-\gamma)}{2\gamma}\right)\Gamma\left(\frac{\pi}{2\gamma}\right)^5} - \frac{5}{3}\cdot\frac{\Gamma\left(\frac{3\pi}{2\gamma}\right)^2\Gamma\left(\frac{\pi-\gamma}{2\gamma}\right)^6}{\Gamma\left(\frac{3(\pi-\gamma)}{2\gamma}\right)^2\Gamma\left(\frac{\pi}{2\gamma}\right)^6} + \frac{15\pi^2\tan^2\left(\frac{\pi^2}{2\gamma}\right)}{(\pi-\gamma)^2} + \frac{5\pi\tan\left(\frac{\pi^2}{2\gamma}\right)}{\pi-\gamma}\cdot\frac{\Gamma\left(\frac{3\pi}{2\gamma}\right)\Gamma\left(\frac{\pi-\gamma}{2\gamma}\right)^3}{\Gamma\left(\frac{3(\pi-\gamma)}{2\gamma}\right)\Gamma\left(\frac{\pi}{2\gamma}\right)^3}\right],$$

5-th order Drude weight diverges for Δ<0 (antiferromagnetic region)

Even-order Drude Weights

Tanikawa-Takasan-Katsura 2021



Vanishes at zero flux by symmetry,
but can be non-vanishing under a non-zero flux and in fact diverges for a range of Δ!

Does the Current Diverge??

Diverging Drude weight does NOT imply
a particularly enhanced current due to nonlinear effects

So far, the divergent nonlinear Drude weights are negative, rather representing the limitation in the linear response current growing linearly in time

The divergent nonlinear Drude weights can be understood in terms of Conformal Field Theory with perturbations
Tanikawa-Takasan-Katsura 2021

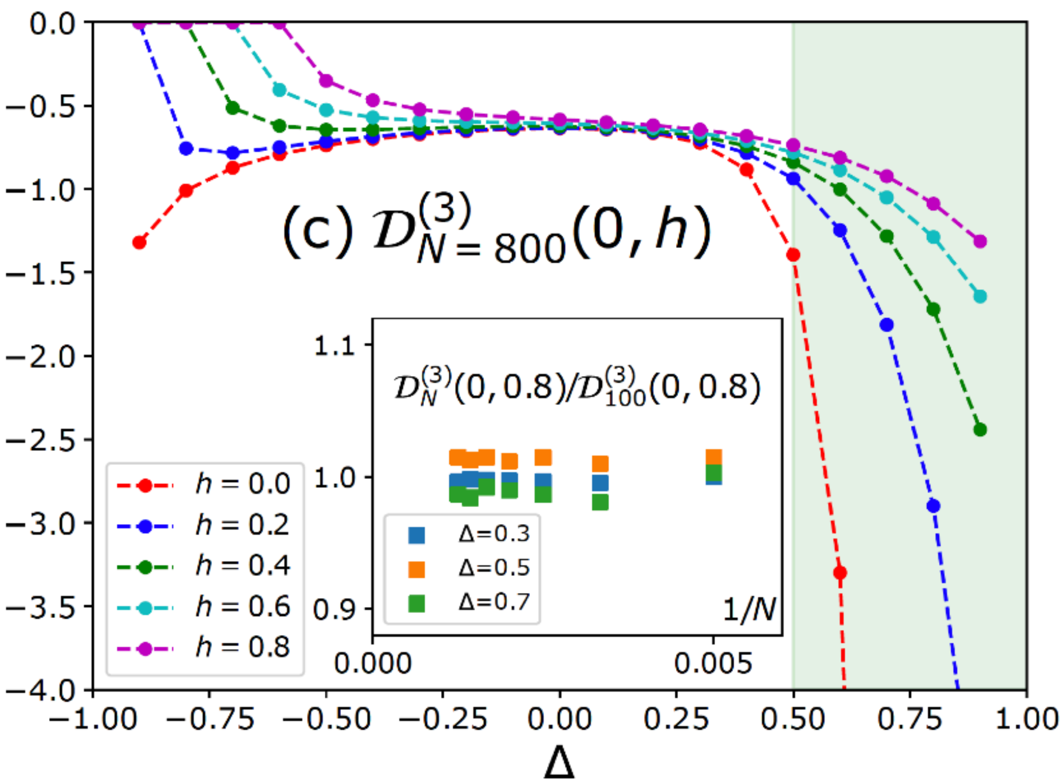
Perturbed Conformal Field Theory

$$e_{\mathrm{gs}}(\Phi) - e_{\mathrm{gs}}(0) = \sum_{k \geq l \geq 1} A_{k,l} \left(\frac{1}{N}\right)^{2k} \Phi^{2l}$$

$$+ \sum_{k,l,m \geq 1} B_{k,l,m} \left(\frac{1}{N}\right)^{2k+4m\frac{\gamma}{\pi-\gamma}} \Phi^{2l},$$

Tanikawa-Takasan-Katsura 2021

Effect of irrelevant perturbations (“Umklapp terms”) to the CFT (Tomonaga-Luttinger Liquid): source of the divergence of the non-linear Drude weights!



magnetic field suppresses the Umklapp terms and thus divergence of the nonlinear Drude weights!

Free Electrons in 1D w/ Defect

K. Takasan, H. Watanabe & M. O. PRB 2023

(with periodic b.c.)

Exactly solvable in terms of the scattering at the defect

$$E_0^{L,\theta} = c_{+1}(\theta)L + c_0(\theta) + c_{-1}(\theta)L^{-1} + o(L^{-1}),$$

$$d_n(\theta) \equiv \frac{d^n c_{-1}(\theta)}{d\theta^n}.$$

L: system size

θ: AB flux (= $A \times L$)

$$\tilde{\mathcal{D}}_{(N)}^{L,\theta} = d_{N+1}(\theta)L^{N-1} + o(L^{N-1}).$$

Nonlinear Drude weight (according to Kohn formula)

diverge if $d_{N+1} \neq 0$!

Why divergent?

Kohn formula: adiabatic limit for a given system size

thermodynamic limit of the Kohn formula:

$L \to \infty$ after $\omega \to 0$

let us call the result as **"Kohn Drude weight"**

But the adiabatic dynamics may require extremely long time scale as the system size is enlarged and may not be physical

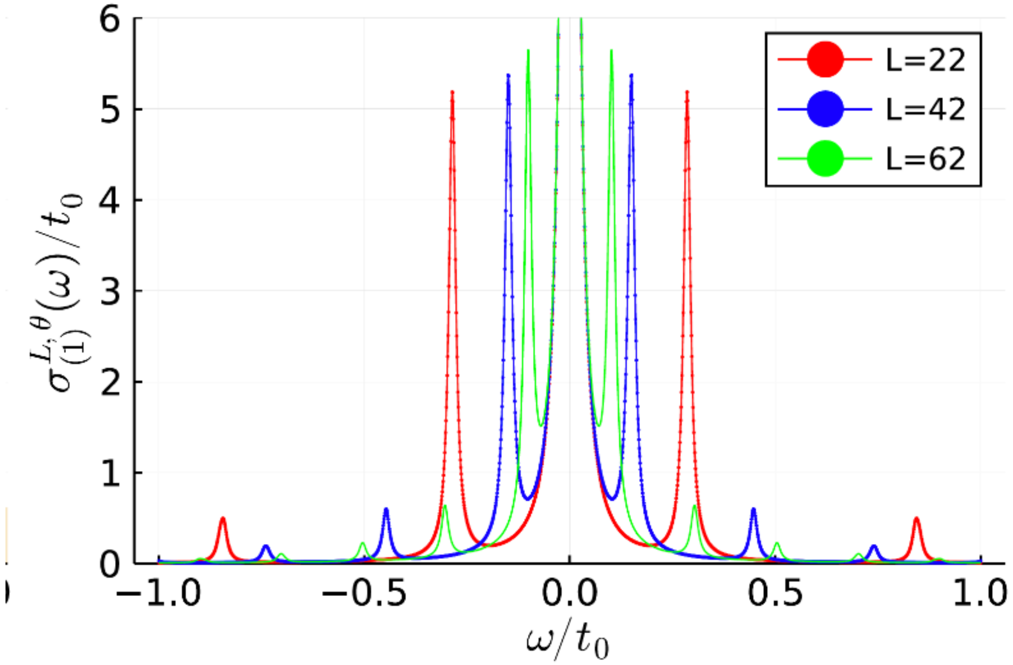
"Bulk Drude weight" may be defined by

$\omega \to 0$ limit after the thermodynamic limit $L \to \infty$

the distinction would be also relevant for linear Drude weights, although the difference is more dramatic for nonlinear Drude weights

Low-Frequency Contributions

(d) $\theta = 1.57$ (Linear conductivity)



low-frequency contributions at ω∼1/*L*

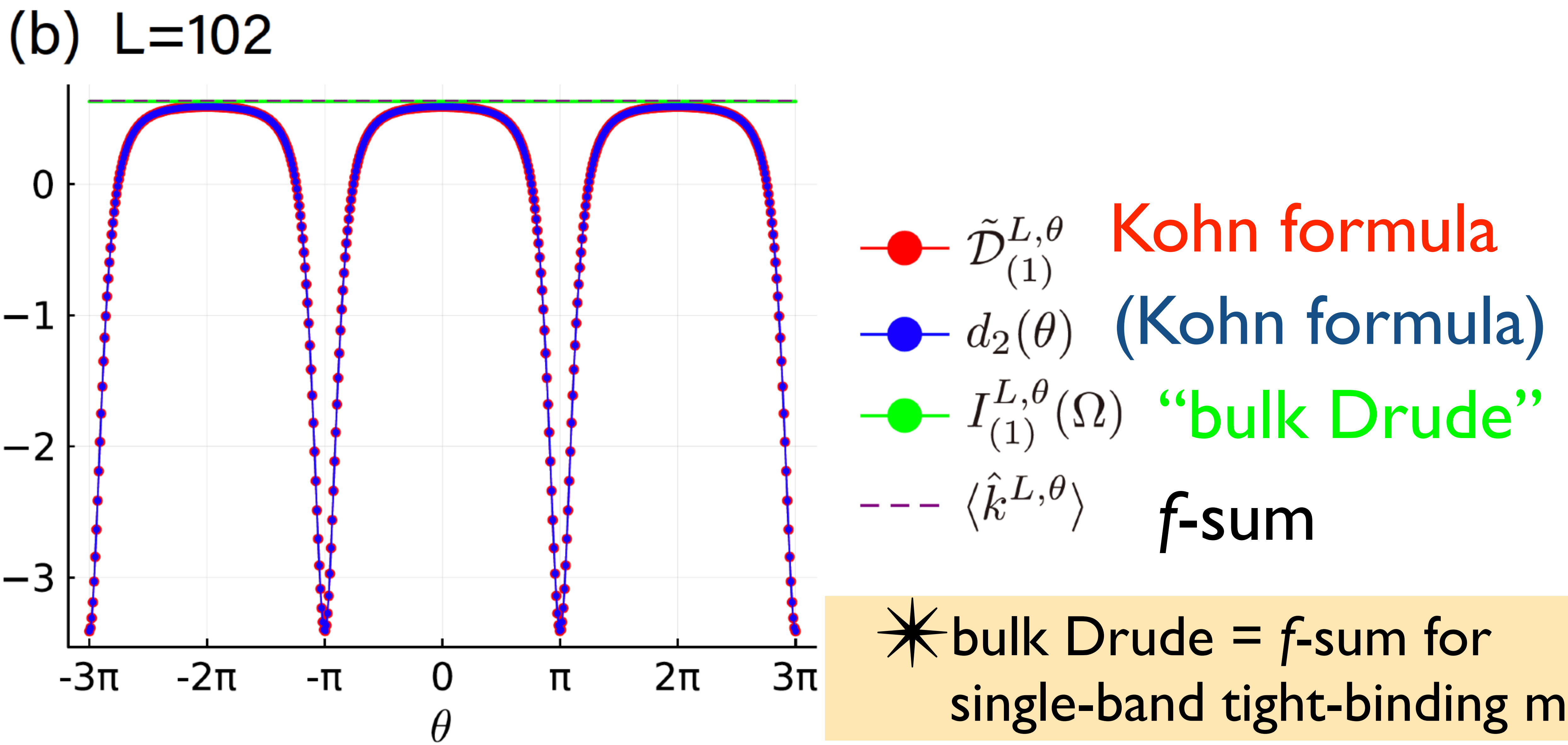
(→ zero frequency in the thermodynamic limit)

Kohn Drude weight: count only strictly ω=0 response for finite *L*

$$I^{L,\theta}_{(N)}(\Omega) \equiv \frac{1}{\pi^N} \int_{-\Omega}^{\Omega} \frac{d\omega_1}{2\pi} \cdots \int_{-\Omega}^{\Omega} \frac{d\omega_N}{2\pi} \sigma^{L,\theta}_{(N)}(\omega_1, \cdots, \omega_N),$$

$$\mathcal{D}^{\mathrm{bulk}}_{(N)} \equiv \lim_{\Omega \to +0} \lim_{L \to \infty} I^{L,\theta}_{(N)}(\Omega),$$

Linear Drude Weight: Kohn vs Bulk

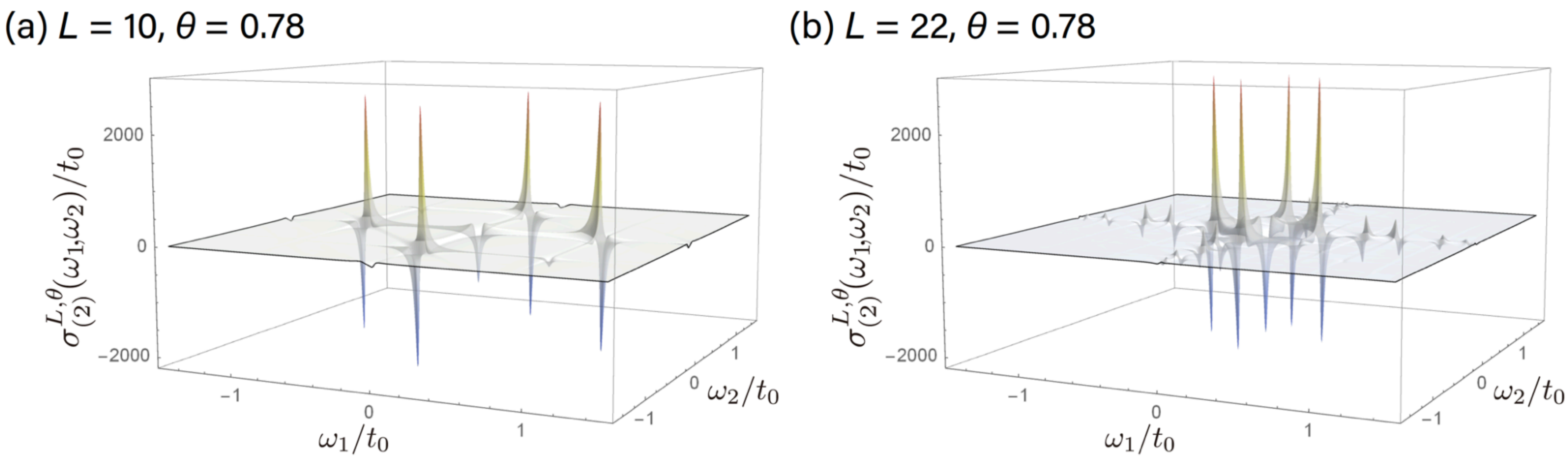


✶bulk Drude = *f*-sum for single-band tight-binding model

Kohn formula: strong dependence on AB flux θ, although the bulk properties should be independent of θ
“bulk Drude weight” including |ω|≦1/L : independent of θ!

Nonlinear Conductivities

e.g.) Second-order conductivity $\sigma^{L,\theta}_{(2)}(\omega_1, \omega_2)$

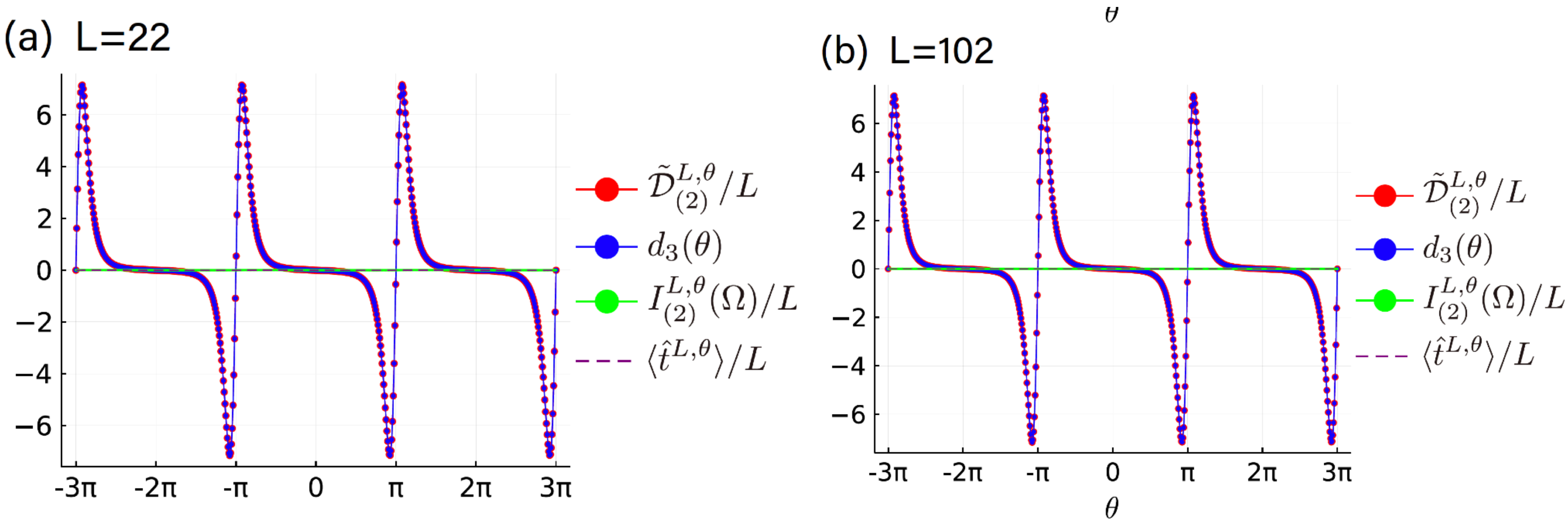


Again we define the "bulk Drude weight" by

$$I^{L,\theta}_{(N)}(\Omega) \equiv \frac{1}{\pi^N} \int_{-\Omega}^{\Omega} \frac{d\omega_1}{2\pi} \cdots \int_{-\Omega}^{\Omega} \frac{d\omega_N}{2\pi} \sigma^{L,\theta}_{(N)}(\omega_1, \cdots, \omega_N),$$

$$\mathcal{D}^{\mathrm{bulk}}_{(N)} \equiv \lim_{\Omega \to +0} \lim_{L \to \infty} I^{L,\theta}_{(N)}(\Omega),$$

2nd order Drude Weights: Kohn vs Bulk



Kohn Drude weight: divergent, depends on AB flux

Bulk Drude weight: finite, independent of AB flux

[actually vanishes cf.) symmetry]

K. Takasan, H. Watanabe & M. O. PRB 2023

Summary

H. Watanabe and M.O., Phys. Rev. B **102**, 165137 (2020)
H. Watanabe, Y. Liu, and M. O., J. Stat. Phys. **181**, 2050 (2020)

***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

Summary II

However, the "Kohn formula" sometimes leads to "pathological" properties unrelated to bulk transport

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

(several works on the linear conductivity, but the problem amplified in the nonlinear conductance)

To probe the bulk property ("bulk Drude weight")
Thermodynamic limit $L \to \infty$ first, then consider "adiabatic limit" $T \to \infty$
$\Leftrightarrow$ $\omega \sim 0$ [coefficient of $\delta(\omega)$] *afterwards*

K. Takasan, H. Watanabe & M. O. PRB **107**, 075141 (2023)

Summary II

M. O. 2003

correct Drude weight. An alternative solution proposed here is to use the real-time formulation (6) instead of the Kohn formula (7). I fix the time interval T (and thus the "sweeping rate" of Φ) and take the thermodynamic limit $L_j \rightarrow \infty$ first. After taking the thermodynamic limit, I let $T \rightarrow \infty$. There could be more and more level crossings and the time evolution is not necessarily adiabatic, as the system size is increased with a fixed T. With huge numbers of crossings in a large system, the final state $|\Psi(T)\rangle$ may actually be very complicated [17] but $\bar{D}$ is still well defined. By taking the $T \rightarrow \infty$ limit after taking the thermodynamic limit, $\bar{D}$ should converge to the standard Drude weight D. This procedure in the real-time corresponds to, in the frequency space, taking the $\omega \rightarrow 0$ limit after taking the thermodynamic limit with $\vec{q} = 0$.

Open Problems

- When Kohn Drude weight = bulk Drude weight ?
- Calculation of bulk Drude weights for interacting systems
- How to utilize the nonlinear *f*-sum rules

etc. etc.