Quantum Quench and $f$-Sum Rules on Linear and Non-linear Conductivities

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Considering a quench process in which an electric field pulse is applied to the system, “$f$-sum rule” for the conductivity for general quantum many-particle systems is derived. It is furthermore extended to an infinite series of sum rules, applicable to the nonlinear conductivity at every order.

Introduction.— Understanding of dynamical responses of a quantum many-body system is not only theoretically interesting but is also essential for bridging theory and experiment, as many experiments measure dynamical responses. Linear responses have been best understood, thanks to the general framework of linear response theory [1]. Many experiments can be actually well described in terms of linear responses. On the other hand, there is a renewed strong interest in nonlinear responses recently, thanks to new theoretical ideas, powerful numerical methods, and developments in experimental techniques such as powerful laser sources which enable us to probe highly nonlinear responses. For example, “shift current”, which is a DC current induced by AC electric field as a higher order effect, has been studied vigorously [2–6]. Yet, theoretical computations of dynamical responses are generally challenging, often even for linear responses and more so for nonlinear ones. Therefore it is useful to obtain general constraints on dynamical responses, including their relations to static quantities which are easier to calculate. The “$f$-sum rule” of the linear electric conductivity is a typical and well-known example of such constraints [7]. For simplicity, here let us consider the uniform component of the linear AC conductivity, which is defined as

$$j_i(\omega) = \sigma_i^{(\text{u})}(\omega) E_j(\omega),$$

where $j_i(\omega) = j_i(-\omega)^*$ is the uniform part ($q = 0$ Fourier component) of the current, $E_j(\omega) = E_j(-\omega)^*$ is the uniform electric field, and $\omega$ is the angular frequency. The $f$-sum rule is a constraint on the frequency integral

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sigma_i^{(\text{u})}(\omega).$$

In condensed matter physics, the Hamiltonian of the following form is often considered:

$$\hat{H} = \hat{K} + \hat{I},$$

where $\hat{K}$ is the kinetic energy (including the chemical potential term) which is bilinear in particle creation/annihilation operators, and $\hat{I}$ is the density-density interaction energy. For the standard kinetic term in non-relativistic quantum mechanics in the continuum

$$\hat{K} = \int dr \hat{\psi}^\dagger(r) \left(-\frac{\nabla^2}{2m} - \mu\right) \hat{\psi}(r),$$

the original form of the $f$-sum rule is known as

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sigma_i^{(\text{u})}(\omega) = \delta_{ij} \frac{\rho}{2m}.$$  (4)

The right-hand side is determined by the electron mass $m$ and the electron density $\rho$, and is a completely static quantity.

For more general models of the form [4], the $f$-sum rule still holds although with a modified right hand side [5–10]. Namely, for a Hamiltonian of the form [2] where the kinetic term is

$$\hat{K} = \int \frac{dp}{(2\pi)^d} \hat{\psi}^\dagger(p) \epsilon(p) \hat{\psi}(p)$$

in the momentum representation, the $f$-sum rule reads

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sigma_i^{(\text{u})}(\omega) = \frac{1}{2} \int \frac{dp}{(2\pi)^d} \left(\hat{\psi}^\dagger(p) \frac{\partial^2 \epsilon(p)}{\partial p_i \partial p_j} \hat{\psi}(p)\right).$$  (6)

In this paper, we relate the $f$-sum rule to a quantum quench process. This picture naturally leads to more general $f$-sum rules than the form [6] that have been discussed in the literature. In particular, we derive an infinite series of “$f$-sum rules” for nonlinear conductivities.

Setup and Result.— We consider a general system of many quantum particles defined on a $d$-dimensional lattice. Let $P$ be the set of lattice points and $L$ be the set of directed links (arrows) connecting a pair of lattice points as shown in Fig. [1](a). We do not require any spatial symmetry such as the translation invariance or the inversion symmetry. The system size and the boundary condition can be chosen arbitrary.

The Hamiltonian $\hat{H}(t)$ of the system is written in terms of creation and annihilation operators $\hat{c}_{x,\alpha}^\dagger, \hat{c}_{x,\alpha}$ ($\alpha$ labels the internal degrees of freedom) defined on each point $x \in P$ and a U(1) vector potential $A_I(t)$ defined on each link $I \in L$, while the scalar potential is set to be 0. The vector potential is introduced as an external field and its time dependence describes the local electric field [17, 18]

$$E_l(t) = \frac{dA_l(t)}{dt}.$$  (7)

We assume that the Hamiltonian is invariant under the local U(1) transformation $\hat{c}_{x,\alpha} \rightarrow e^{i\theta_{x,\alpha}} \hat{c}_{x,\alpha}$ and
A \tilde{l}_{ij}(t) \rightarrow A \tilde{l}_{ij}(t) - \delta \tilde{x}_j + \theta \tilde{x}_i, \text{ where the link } \tilde{l}_{ij} \in L \text{ goes from } \tilde{x}_i \in P \text{ to } \tilde{x}_j \in P. \text{ This enables us to define the conserved current density}
\[ \hat{\nu}_l(t) = \frac{\partial \hat{H}(t)}{\partial A_l(t)} \]  
(8)

at every link. We allow any number of creation and annihilation operators to appear in a single term in the Hamiltonian, representing correlated hopping, pair hopping, ring exchange, and so on. We assume that all the hoppings and interactions are short-ranged and that the Hamiltonian depends on \( t \) only through \( A_l(t) \) [19].

Suppose that the system is described by a density operator \( \hat{\rho}(0) \) at \( t = 0 \). The evolution of the system is given by the time-evolution operator \( \hat{S}(t) \) defined by

\[ \frac{d\hat{S}(t)}{dt} = -i\hat{H}(t)\hat{S}(t), \quad \hat{S}(0) = 1. \]  
(9)

The expectation value of any operator \( \hat{\Omega}(t) \) at time \( t \) is then given by
\[ \langle \hat{\Omega}(t) \rangle_t \equiv \text{Tr}[\hat{\Omega}(t)\hat{S}(t)\hat{\rho}(0)\hat{S}(t)\dagger]. \]  
(10)

The linear and nonlinear conductivities in real space and time are defined as the response of the local current density as a result of the applied electric field:

\[ \langle \hat{\nu}_l(t) \rangle_t = \langle \hat{\nu}_l(0) \rangle_0 \]
\[ + \sum_{m \neq 0} \int_0^t dt' \sigma_l^m(t, t') \prod_{\nu \in L} \frac{1}{m_{\nu'}!} \prod_{i=1}^{m_{\nu'}} E_{\nu'}(t'_{\nu'}). \]  
(11)

Here, \( t' \) is the collection of \( t_{\nu'} \) and \( \int_0^t dt' \equiv \prod_{\nu \in L} \prod_{i=1}^{m_{\nu'}} \int_0^{t_{\nu'}} dt'_{\nu'} \) is the convolution integral. Also, \( m \) is the collection of \( m_l \geq 0 \) and
\[ N \equiv \sum_l m_l \]  
(12)

represents the order of responses. Namely, \( \sigma_l^m(t, t') \) with \( N = 1 \) represents the (spatially-resolved) linear conductivity, whereas the case with \( N \geq 2 \) corresponds to nonlinear conductivities.

Our main result of this work is the following constraint on instantaneous conductivities for any \( m \neq 0 \):
\[ \sigma_l^m(0, 0) = \langle \hat{H}^m|_{m_l \rightarrow m_l+1} \rangle_0, \]  
(13)
\[ \hat{H}^m \equiv \prod_{l \in L} \frac{\partial^{m_l}}{\partial A_l(t)^{m_l}} \hat{H}(t)|_{t=0}. \]  
(14)

In Eq. \[13\], \( \sigma_l^m(0, 0) \) is the shorthand for
\[ \lim_{t \to +0} \lim_{t' \to +0} \sigma_l^m(t, t') \]  
(15)

and \( m_l \rightarrow m_l + 1 \) means replacing \( m_l \) in \( m \) with \( m_l + 1 \). This spatially-resolved formula implies, among other things, that the instantaneous response for short-range hopping models vanishes when \( l \) and \( l' \) are sufficiently apart. This is consistent with the intuition, and also with the Lieb-Robinson bound [20].

The constraint \[13\] is valid on the instantaneous response in an arbitrary initial state \( \hat{\rho}(0) \). A natural choice of \( \hat{\rho}(0) \) would be an equilibrium density matrix (Gibbs state) at a certain temperature, but \( \hat{\rho}(0) \) can also be chosen to represent a non-equilibrium state [21, 22], especially a non-equilibrium steady state for which the response function would still be time-translation invariant [23]. In a steady state including the equilibrium, \( \sigma_l^m(t, t') \) depends only on the time differences \( \Delta t_{\nu'} = t - t'_{\nu'} \). In such a case, it is common to work in the frequency space after a Fourier transformation on \( \Delta t_{\nu'} \). Then the left hand side of Eq. \[13\] reads
\[ \sigma_l^m(0, 0) = 2^N \int_{-\infty}^{\infty} d\omega \sigma_l^m(\omega), \]  
(16)

where \( \omega \) is the collection of \( \omega_{\nu'} \) and \( \int_{-\infty}^{\infty} d\omega = \prod_{\nu \in L} \prod_{i=1}^{m_{\nu'}} \int_{-\infty}^{\infty} \frac{d\omega_{\nu'}}{2\pi} \). The factor \( 2^N \) originates from the discontinuity of \( \sigma_l^m \) around \( \Delta t_{\nu'} = 0 \). Eqs. \[13\] and \[16\] give general, position-dependent \( f \)-sum rules in terms of the frequency integral.

Example: uniform response on square lattice.— To illustrate implications of our result in the simplest setting, let us take the 2D square lattice and discuss the response of the averaged current density toward a uniform electric field. We assign the common value of the vector potential \( A_2(\tilde{x}) \) (or \( A_y(\tilde{x}) \)) to the horizontal (vertical) links in Fig. 1 (b). In this case, the averaged current density is defined by
\[ \hat{\nu}_l(t) = \frac{1}{V} \frac{\partial \hat{H}(t)}{\partial A_l(t)} \quad (i = x, y) \]  
(17)

(\( V \) is the volume of the system) and the definition of
conductivities in Eq. \[11\] is simplified to
\[
\hat{\jmath}(t)_{l} = \hat{\jmath}(0)_{0},
\]
\[
+ \int_{t}^{0} dt_{1} \left[ \sigma_{x}^{(0)}(0,0) \right]_{t=0},
\]
\[
+ \int_{t}^{0} dt_{1} \int_{t}^{0} dt_{2} \left[ \frac{1}{2} \sigma_{x}^{(0)}(0,0) \right]_{t=0}.
\]
Our result \[13\] reproduces the well-known f-sum rule on the linear conductivity \[22\]:
\[
\sigma_{x}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{x}}|_{t=0},
\]
\[
\sigma_{y}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{y}}|_{t=0},
\]
\[
\sigma_{x}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{x}}|_{t=0},
\]
\[
\sigma_{y}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{y}}|_{t=0}.
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\[
\sigma_{x}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{x}}|_{t=0}.
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\sigma_{y}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{y}}|_{t=0}.
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\]
\[
\sigma_{y}^{(0)}(0,0) = \frac{1}{2V} \frac{\partial \tilde{H}}{\partial A_{y}}|_{t=0}.
\]
Derivation of the Main Result.—To demonstrate our result \[13\], we choose the vector potential on the link \(l\) to be
\[
A_{l}(t) = f_{l}(t/T), \quad A_{l},
\]
where \(A_{l}\) is a constant and \(f_{l}(\tau)\) is a smooth function satisfying \(f_{l}(\tau) = 0\) for \(\tau < 0\) and \(f_{l}(\tau) = 1\) for \(\tau > 1\).
We start with verifying
\[
\frac{d}{dt}(\hat{H}(t))_{l} = \frac{\delta \hat{H}}{\delta A_{l}} \frac{dt}{dt},
\]
by combining Eqs. \[7\]-\[10\]. Integrating this equation over \(t \in [0, T]\), we get
\[
\langle \hat{H}(T) \rangle_{l} - \langle \hat{H}(0) \rangle_{l} = \sum_{l \in L} \int_{0}^{T} dt E_{l}(t) \langle \hat{\jmath}(t) \rangle_{l}.
\]
A relation similar to \[29\] for the uniform current and electric field was used in Ref. \[25\]. There, the limit \(T \to \infty\) of the adiabatic flux insertion was considered, in order to discuss the Drude weight at zero temperature \(\beta \to \infty\). The adiabatic insertion leads to the famous Kohl formula for the Drude weight \[26\]. However, the formula \[29\] is valid for general \(T\) and for any initial state. Here we consider the opposite limit, that is the limit of very quick insertion of flux: \(T \to 0\). This can be regarded as an example of quantum quench (sudden switching of the vector potential). In this limit, the state cannot follow the change of the Hamiltonian, and “the sudden approximation \(\tilde{S}(t) = 1\)” becomes exact \[27\]. This can be most easily seen by the formula \(T\) denotes the time-ordering
\[
\tilde{S}(t) = Tr e^{-i t \sum_{m}^{L} \frac{H}{m_{l}} \int_{0}^{T} dt H[\hat{\jmath}(t), A_{l}]}.
\]
Because of the prefactor \(T\) in the exponent, \(\tilde{S}(t) \to 1\) in the limit of \(T \to 0\) for any \(0 \leq t \leq T\). In this limit, only the “diamagnetic” contributions survive in the current response.
In the following, we expand each side of Eq. \[29\] into the power series of \(A_{l}\) in the quench limit \(T \to 0\). On the one hand, the left-hand side of Eq. \[29\] is reduced to \(\langle \hat{H}(T) - \hat{H}(0) \rangle_{l}\), which admits the Taylor expansion
\[
\langle \hat{H}(T) - \hat{H}(0) \rangle_{l} = \sum_{m_{l}=0}^{d} \frac{1}{m_{l}} A_{l}^{m_{l}}.
\]
On the other hand, we approximate \(\sigma_{x}^{l}(m, l)\) in Eq. \[11\] by \(\sigma_{x}^{m}(0, 0)\) assuming that \(T\) is small enough. We can then easily perform the \(\int_{0}^{T} dt l\) integral and get
\[
\langle \hat{\jmath}(t) \rangle_{l} = \langle \hat{\jmath}(0) \rangle_{0} + \sum_{m_{l} \neq 0} \frac{1}{m_{l}} A_{l}^{m_{l}},
\]
Thus the right-hand side of Eq. \[29\] becomes
\[
\sum_{l \in L} \int_{0}^{T} dt E_{l}(t) \langle \hat{\jmath}(t) \rangle_{l} = \sum_{l \in L} A_{l} \langle \hat{\jmath}(0) \rangle_{0} + \sum_{m_{l}} \sum_{m_{l} \geq 1} \frac{1}{m_{l}} A_{l}^{m_{l}}.
\]
(33)
where
\[ I_l^m \equiv \int_0^1 dt \partial_\tau |f_I(\tau)|^m \prod_{l' \neq l} |f_{l'}(\tau)|^{m_{l'}}. \] (34)

When \( m_l = 0 \), \( \sigma_l^{m_l \rightarrow m_l-1}(0,0) \) is ill-defined but in this case \( I_l^m \) vanishes and Eq. (35) still holds.

Matching the coefficient of \( \prod_{l \in L} \gamma_{l}^{A_{l}} \) in Eqs. (31) and (33), we find
\[ \langle \hat{H}^m \rangle_0 = \sum_{l \in L} \sigma_l^{m_l \rightarrow m_l-1}(0,0) I_l^m \] (35)

for \( N \geq 2 \). Note that the integral \( I_l^m \) depends on the specific choice of the function \( f_I(\tau) \). To avoid contradiction, we demand the invariance of the right-hand side of Eq. (35) under an arbitrary variation \( \delta f_I(\tau) \) with \( \delta f_I(0) = \delta f_{I}(1) = 0 \). It implies
\[ \sigma_l^{m_l \rightarrow m_l-1}(0,0) = \sigma_{l'}^{m_{l'} \rightarrow m_{l'}-1}(0,0) \] (36)

for any pairs of \( l \) and \( l' \) with \( m_l \geq 1 \) and \( m_{l'} \geq 1 \). Plugging this relation back to Eq. (35) and using \( \sum_{l \in L} I_l^m = \int_0^1 dt \partial_\tau \prod_{l \in L} \gamma_{l}^{A_{l}} = 1 \), we recover our main result in Eq. (13).

Discussion.— In this work, we obtained an infinite series of sum rules on the nonlinear conductivities, although just one sum rule for \( \sigma_l^m \), which has multiple arguments, was found. We stress that the present approach is quite general and not limited to the Hamiltonians \( \hat{H}^m \). It can be also naturally understood that the density-density interactions do not appear explicitly in the sum rule: any term in Hamiltonian which does not couple to the gauge field does not contribute to \( H^m \).

While we used lattice models in our derivation, essentially the same argument applies to continuum models as well. For the particular case of the nonrelativistic quantum mechanical Hamiltonian \( \hat{H}^m \) with \( \hat{L}^m \), the right-hand side of the main result, Eq. (13), vanishes for nonlinear conductivities. Although this is rather remarkable, this does not imply the absence of a nonlinear current response to the electric field. Eq. (13) just represents the instantaneous response, and even when it vanishes, the response can be non-vanishing at a later time. In the frequency representation \( \tilde{\alpha}(\omega) \), the vanishing of Eq. (13) implies that any positive part of \( \sigma_l^m(\omega) \) must be compensated by a negative part.

The present result is one of rather few general constraints on conductivities, especially non-linear ones. The sum rules can be used to check various approximations or numerical calculations, and might give a guiding principle on designing systems with desired transport properties. We hope that the present result will help developing theory of linear and nonlinear dynamical responses of quantum many-body systems in the future.

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[23] We thank Kazuaki Takasan for suggesting potential applications to non-equilibrium steady states.

[24] In Ref. [10], a breakdown of the sum rule for the uniform $q = 0$ component was discussed. However the issue is presumably related to the subtlety of the Drude peak. In the perfectly periodic system studied in the present paper, at least in a finite-size system, the sum rule is exactly satisfied by including the possible Drude peak in the integral, as implied by the argument presented in the main text.

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[27] The fact that $\hat{S}(t) \rightarrow 1$ in the $T \rightarrow 0$ limit might sound puzzling, since the applied electric field may still give a non-zero impulse to the system even in the quench limit. This is not a contradiction because the impulse is not described by $\hat{S}(t)$ but by the (large) gauge transformation that brings $\hat{H}(T)$ back to $\hat{H}(0)$, although here we do not perform such a transformation.