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Positivity of the spectral densities of retarded Floquet Green functions

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Periodically driven nonequilibrium many-body systems are interesting because they have a quasi-energy spectra, which can be tailored by controlling the external driving fields. We derive the general spectral representation of retarded Green functions in the Floquet regime, thereby generalizing the well-known Lehmann representation from equilibrium many-body physics. The derived spectral Floquet representation allows us to prove the nonnegativity of spectral densities and to determine exact spectral sum rules, which can be employed to benchmark the accuracy of approximations to the exact Floquet many-body Green functions.

Nonequilibrium many-body physics is a vibrant field, both from the experimental and from the theoretical side. Largely, this has been triggered by the ease with which one can tune and manipulate the time dependence of systems of ultracold atoms in optical lattices [1, 2]. But there also have been significant advances in solid state systems, which employ ultrafast pump-probe techniques to study electrons on femto-second timescales [3–5].

Periodically driven many-body systems are simpler than general nonequilibrium systems, because the Hamiltonian repetitively cycles through the same functional form again and again. Conceptually, Floquet theory for periodic linear differential equations (and also periodic Hamiltonians) [6–8] is a powerful tool to treat these periodically modulated quantum systems. One fundamental development is the notion of Floquet design, i.e., the possibility to engineer quantum systems with certain desired properties, e.g., with topological phases [9], by properly selecting the external drive, see, e.g., Refs. 10–13. An important issue for experimentally realizing such systems is how long the system has to be driven to display Floquet-like behavior [14]? It turns out that the drive time need not be so long for many of these systems, as has been experimentally demonstrated with topological insulators [15].

In spite of the large interest in periodically driven many-body systems, rigorous statements about the properties of measurable and computable quantities in the Floquet regime are scarce. As a relevant example, we draw the reader's attention to the fact that the fermionic spectral density is nonnegative in equilibrium, allowing its interpretation as a probabilistic density of states. But in Floquet systems, there is no *a priori* guarantee that a spectral density will be nonnegative. As a result, others have employed weighted sums over various elements of the response functions in the Floquet representation [12, 16–18], which have turned out to be nonnegative. But to our knowledge, no proof of nonnegativity has been offered. This is a nontrivial issue, as the standard approach to constructing spectral functions, which involves using Wigner coordinates of average and relative time,

and Fourier transforming the relative time to a frequency, produces spectral functions $A(\omega, t_{\text{ave}})$ that usually display negative values. However, they become nonnegative after further averaging over t_{ave} [14, 19, 20]. For noninteracting single-band models, analytical proofs do exist that show how averaging over one period T guarantees nonnegative spectral densities [14, 21]. Nevertheless, negative densities are sometimes seen for interacting systems [21], so far without explanation. This illustrates the need for tangible analytic results which hold also in presence of interactions.

We solve this problem by deriving a spectral representation for retarded Green functions in the quasi-stationary Floquet regime. This spectral representation generalizes the well-established Lehmann representation of equilibrium quantum mechanics. Like the latter, our generalization allows one to derive rigorous general conclusions, e.g., on the nonnegativity of spectral functions and on their sum rules. For this reason, the derived results will guide many future studies in the field.

We consider a closed quantum-mechanical system described by the time-dependent periodic Hamiltonian

$$\mathcal{H}(t) = \mathcal{H}(t + T) \quad \forall t, \quad (1)$$

where T is the temporal period. Hence, any linear-response function, e.g., a fermionic or bosonic propagator, generically depends on two times t_1 and t_2 in a nontrivial way. In other words, the relative time t_{rel} alone is not sufficient, in contrast to time-invariant systems with constant Hamiltonians $\partial_t \mathcal{H} = 0$, where only the relative time dependence enters.

Wigner's prescription for the relative and average times is given by

$$t_{\text{rel}} := t_1 - t_2 \quad (2a)$$

$$t_{\text{ave}} := (t_1 + t_2)/2. \quad (2b)$$

Kubo's formalism tells us that a retarded Green function satisfies

$$G(t_1, t_2) := -i \left\langle [c(t_1), c^\dagger(t_2)]_{\pm} \right\rangle \Theta(t_1 - t_2), \quad (3)$$

where c can be any, possibly composite, fermionic or bosonic operator, e.g., a fermionic annihilation operator in position space or in momentum space or a Hubbard operator. If it is overall fermionic (that means odd in the number of fermionic creation or annihilation operators), then the $+$ sign applies in the anticommutator $[\cdot]_+$; if it is overall bosonic, then the $-$ sign applies in the commutator $[\cdot]_-$. We re-express $G(t_1, t_2)$ in terms of t_{rel} and t_{ave} and transform the dependence on t_{rel} to frequency space

$$G(\omega, t_{\text{ave}}) := \lim_{\delta \rightarrow 0^+} \int_0^\infty e^{i(\omega + i\delta)t_{\text{rel}}} G(t_{\text{ave}} + t_{\text{rel}}/2, t_{\text{ave}} - t_{\text{rel}}/2) dt_{\text{rel}}. \quad (4)$$

We are interested in the spectral function $A(\omega, t_{\text{ave}})$, which we define by the negative imaginary part of the retarded Green function $A(\omega, t_{\text{ave}}) := -\text{Im}G(\omega, t_{\text{ave}})/\pi$ as usual. We will derive a spectral representation for the Wigner representation [21, 22] of this quantity below. For clarity, we deal with the greater Green function $G^>(t_1, t_2) := -i\langle c(t_1)c^\dagger(t_2) \rangle$ [23] in the explicit calculations; the expressions for the lesser Green function $G^<(t_1, t_2) := \pm i\langle c^\dagger(t_2)c(t_1) \rangle$ (the upper sign refers to fermions) are analogous. Finally, we are interested in the retarded Green function $G(t_1, t_2) = (G^>(t_1, t_2) - G^<(t_1, t_2))\Theta(t_1 - t_2)$ [24] in order to define the spectral densities. Note that we expect there to be stronger average time dependence to the lesser and greater Green functions (due to heating effects) than to the retarded Green function, since the latter is determined primarily by the quantum states and not by how those states are occupied.

For comparison, it is useful to recall the Lehmann representation for a time-independent Hamiltonian \mathcal{H} . Let us assume that $\{|m\rangle\}$ is an eigenbasis of \mathcal{H} with eigenvalues $\tilde{\epsilon}_m$ and that the system is in the state $|m\rangle$ with probability $p_m \geq 0$ and $\sum_m p_m = 1$. We do not necessarily require a thermal distribution $p_m \propto \exp(-\beta\tilde{\epsilon}_m)$ for these probabilities, but we do require monotonicity for the bosonic case, where $p_m \geq p_n$ if $\tilde{\epsilon}_m \leq \tilde{\epsilon}_n$. Then the greater Green function can be expressed as

$$G^>(t_1, t_2) = -i \sum_{m,n} p_m |\langle m|c|n\rangle|^2 e^{i(\tilde{\epsilon}_m - \tilde{\epsilon}_n)t_{\text{rel}}}. \quad (5)$$

The Fourier transform of Eq. (4) of the retarded Green function leads to

$$A(\omega) = \sum_{m,n} (p_m \pm p_n) |\langle m|c|n\rangle|^2 \delta(\omega - (\tilde{\epsilon}_n - \tilde{\epsilon}_m)), \quad (6)$$

which does not depend on t_{ave} because \mathcal{H} is time-independent. Recall that $A(\omega)$ is strictly nonnegative in the fermionic case and in the bosonic case for $\omega \geq 0$ since $\tilde{\epsilon}_n \geq \tilde{\epsilon}_m$ implies $p_n \leq p_m$ (due to our monotonicity requirement); for bosons and $\omega \leq 0$, $A(\omega)$ is nonpositive.

For periodic Hamiltonians, the Schrödinger equation $i\partial_t|\psi(t)\rangle = \mathcal{H}(t)|\psi(t)\rangle$ is generally solved by the linear superposition of special solutions of the form [7, 8]

$$|\psi_m(t)\rangle = \exp(-i\epsilon_m t)|m, t\rangle \quad \forall m \in \mathbb{N}_0 \quad (7)$$

where the Floquet states $|m, t\rangle$ are periodic in time with period T $|m, t + T\rangle = |m, t\rangle$. **Different from the eigen-value $\tilde{\epsilon}_m$ in equilibrium, the quasi-energy ϵ_m is uniquely defined only if it is restricted to the interval $\epsilon_m \in (-\pi/T, \pi/T]$.** This ansatz strongly reminds of the Bloch theorem transferred to time. At any given instant t , the states $|m, t\rangle$ form a complete, orthonormal basis. Hence, the unitary time evolution $U(t_1, t_2)$ from time t_2 to time t_1 is expressed by

$$U(t_1, t_2) = \sum_{m=0}^{\infty} \exp(-i\epsilon_m(t_1 - t_2)) |m, t_1\rangle\langle m, t_2| \quad (8)$$

which we will use next. These properties are derived in the Supplementary Material [25].

Now we derive the spectral representation in terms of the Floquet states $|m, t\rangle$. Using $U(t_1, t_2)$ and assuming that the system was at some time t_0 in the Floquet state $|m, t_0\rangle$ with probability p_m , we obtain for the greater Green function

$$G^>(t_1, t_2) = -i \sum_{m=0}^{\infty} p_m \langle m, t_0|U(t_0, t_1)cU(t_1, t_2)c^\dagger U(t_2, t_0)|m, t_0\rangle. \quad (9)$$

Inserting the result in Eq. (8) yields

$$G^>(t_1, t_2) = -i \sum_{m,n=0}^{\infty} p_m e^{-i\epsilon_m(t_0 - t_1)} \langle m, t_1|c|n, t_1\rangle e^{-i\epsilon_n(t_1 - t_2)} \langle n, t_2|c^\dagger|m, t_2\rangle e^{-i\epsilon_m(t_2 - t_0)}. \quad (10)$$

The dependence on t_0 cancels out so that one may choose any appropriate instant. We define the T -periodic functions

$$\Phi_{m,n}(t) := \langle m, t|c|n, t\rangle \quad (11)$$

so that $\Phi_{m,n}^*(t) = \langle n, t|c^\dagger|m, t\rangle$, and we can express Eq. (10) by

$$G^>(t_1, t_2) = -i \sum_{m,n=0}^{\infty} p_m e^{i(\epsilon_m - \epsilon_n)t_{\text{rel}}} \Phi_{m,n}(t_1)\Phi_{m,n}^*(t_2). \quad (12)$$

This result strongly resembles Eq. (5), but cannot be Fourier transformed directly due to the time dependence of the functions $\Phi_{m,n}(t)$. But the latter can be represented by a *Fourier series* due to its time-periodicity

$$\Phi_{m,n}(t) = \sum_{\alpha \in \mathbb{Z}} f_{m,n}^{(\alpha)} e^{i\alpha\Omega t}, \quad (13)$$

where $\Omega = 2\pi/T$. Inserting this expression (and its complex conjugate) into the Wigner representation of the modified greater Green function yields

$$\tilde{G}_\ell^>(\omega) := \int_0^\infty dt_{\text{rel}} e^{i\omega t_{\text{rel}}} \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} dt_{\text{ave}} e^{i\ell\Omega t_{\text{ave}}} \tilde{G}^>(t_1, t_2). \quad (14)$$

Here, the modified greater Green function has an additional $\Theta(t_{\text{rel}})$ multiplied in to allow us to produce the retarded Green function. The two integrals can be done, and yield

$$G_\ell^>(\omega) = \sum_{m,n=0}^\infty p_m \sum_{\alpha \in \mathbb{Z}} f_{m,n}^{(\alpha)} f_{m,n}^{(\alpha+\ell)*} \left\{ \frac{P}{\Delta\epsilon} - i\pi\delta(\Delta\epsilon) \right\} \quad (15a)$$

where P stands for the principal value of the pole and

$$\Delta\epsilon := \omega - (\epsilon_n - \epsilon_m) + (\alpha + \ell/2)\Omega. \quad (15b)$$

If we combine this result with the analogous result for the similarly modified lesser Green function $\tilde{G}^<$ one obtains the Fourier coefficients of the Fourier series of the retarded spectral function $A(\omega, t_{\text{ave}}) = \sum_{\ell \in \mathbb{Z}} A_\ell(\omega) \exp(-i\ell\Omega t_{\text{ave}})$

$$A_\ell(\omega) = -\frac{1}{\pi} \text{Im} G_\ell(\omega) \quad (16a)$$

$$= \sum_{m,n=0}^\infty (p_m \pm p_n) \sum_{\alpha \in \mathbb{Z}} f_{m,n}^{(\alpha)} f_{m,n}^{(\alpha+\ell)*} \delta(\Delta\epsilon), \quad (16b)$$

where $+$ refers to fermionic operators and $-$ to bosonic ones. This equation yields the general spectral representation of Floquet response functions; it generalizes the Lehmann representation in equilibrium and is the key result of our Letter.

What can be deduced from Eq. (16)? For $\ell \neq 0$ we do not see any possibility for a general conclusion on positivity or reality of the spectral function. But for $\ell = 0$, it is obvious that

$$A_0(\omega) = \sum_{m,n=0}^\infty (p_m + p_n) \sum_{\alpha \in \mathbb{Z}} \left| f_{m,n}^{(\alpha)} \right|^2 \delta(\omega - \epsilon_n + \epsilon_m + \alpha\Omega) \quad (17a)$$

$$\geq 0 \quad (17b)$$

in the fermionic case, i.e., $A_0(\omega)$ is nonnegative and can be interpreted as a density-of-states just like in equilibrium. This conclusion is closely related to Bochner's theorem [26]. Note that no general conclusion is possible in the bosonic case since the interplay of the factor $(p_m - p_n)$ and the shift $\alpha\Omega$ can be complicated. We stress that the case $\ell = 0$ corresponds precisely to the average of $A(\omega, t_{\text{ave}})$ over one period of t_{ave} as we used previously [14] to reach physically meaningful results in the noninteracting case. Other authors have also averaged over one period to avoid negative spectral densities [19, 20],

but without explaining why the results must be nonnegative. The above derivation puts this averaging procedure on a firm mathematical basis.

Sum rules are another useful spin-off from spectral representations. Using Eq. (16), we consider the zeroth-moment sum rule S and obtain

$$S := \int_{-\infty}^\infty A_0(\omega) d\omega \quad (18a)$$

$$= \sum_{m,n=0}^\infty (p_m \pm p_n) \sum_{\alpha \in \mathbb{Z}} \left| f_{m,n}^{(\alpha)} \right|^2 \quad (18b)$$

$$= \frac{1}{T} \sum_{m,n=0}^\infty (p_m \pm p_n) \int_t^{t+T} |\Phi_{m,n}(t')|^2 dt' \quad (18c)$$

where the last step results from Parseval's identity. Reinserting the definition from Eq. (11) for $\Phi_{m,n}(t)$ and using the completeness relation [25] $\mathbb{1} = \sum_n |n, t\rangle \langle n, t|$, we arrive at the general sum rule

$$S = \frac{1}{T} \sum_m p_m \int_t^{t+T} \langle m, t' | [c, c^\dagger]_\pm | m, t' \rangle dt' \quad (19)$$

which is consistent with the value of $G(t+0, t)$ in (3) averaged over one period T . While in equilibrium, the sum rule is given by the expectation value of the (anti)commutator for (fermionic) bosonic operators, it is given by the temporal average in the Floquet regime. Hence, we find tangible evidence that the equivalent of a constant expectation value or a constant spectral density at equilibrium is the temporal average of such an expectation value or of such a spectral function, respectively. The sum rules for higher moments of the spectral densities are commutators of products of operators in time so that they become convolutions after Fourier transformations in Floquet representation. Examples of such sum rules are given in the Supplementary Material [25].

The sum rule in Eq. (19) is particularly meaningful if we consider fermionic or bosonic single-particle propagators, i.e., c is a single-particle annihilation operator and c^\dagger the corresponding creation operator. Then, every expectation value on the right hand side equals unity and so does the temporal average and the weighted sum. Hence, the sum rule is indeed rigorously the same as in equilibrium for the averaged spectral functions. We then conclude that a fermionic spectral density in the Floquet regime can be interpreted to be a density-of-states similar to what happens in equilibrium. This has been used already in many numerical studies, see for instance Refs. 17, 18, and 21.

Finally, we transform from the Wigner representation to the often employed equivalent Floquet representation. They are related by

$$G_{\ell_j}(\omega) := G_{\ell-j}(\omega + \Omega(\ell + j)/2), \quad (20)$$

where $\ell, j \in \mathbb{Z}$ according to Tsuji et al. [21]. It is obvious that the Floquet representation does not contain more

information than the Wigner representation. Indeed, the Floquet representation is redundant unless one restricts its argument ω to the interval $(-\Omega/2, \Omega/2]$ [21], but this restriction is not needed otherwise. Equation (20) implies that the physically meaningful time-averaged Green functions appearing in the Wigner representation at index zero occur in the Floquet representation along the diagonal, i.e., for $\ell = j$. One has $G_{\ell\ell}(\omega) = G_0(\omega + \ell\Omega)$ where different indices ℓ correspond to different shifts relative to G_{00} . This Green function and the spectral density $A_0(\omega)$ stemming from its imaginary part are generically used [17, 18, 21] because they behave like equilibrium spectral densities. The negative spectral densities found in Ref. 21 for the gauge-invariant Green function are due to the gauge-invariant transformation, which can no longer be proven to be nonnegative.

For completeness, we also provide the general expression for the nondiagonal Floquet spectral functions $A_{\ell j}(\omega) = -\text{Im}G_{\ell j}(\omega)/\pi$ which reads

$$A_{\ell j}(\omega) = \sum_{m,n=0}^{\infty} (p_m \pm p_n) \sum_{\alpha \in \mathbb{Z}} f_{m,n}^{(\alpha-l)} f_{m,n}^{(\alpha-j)*} \times \delta(\omega - (\epsilon_n - \epsilon_m) + \alpha\Omega). \quad (21)$$

This expression helps to understand why one obtains a positive spectral function upon summing over all Floquet indices ℓ and j as done in Ref. 16. Clearly

$$A_{\Sigma}(\omega) := \sum_{\ell, j \in \mathbb{Z}} A_{\ell j}(\omega) \quad (22a)$$

$$= \sum_{m,n=0}^{\infty} (p_m \pm p_n) |F_{m,n}|^2 \sum_{\alpha \in \mathbb{Z}} \delta(\omega - \epsilon_n + \epsilon_m + \alpha\Omega) \quad (22b)$$

which also yields a nonnegative spectral density with

$$F_{m,n} := \sum_{\ell \in \mathbb{Z}} f_{m,n}^{(\ell)} = \Phi_{m,n}(t=0). \quad (23)$$

Note that no dependence on α remains except a shift by $\alpha\Omega$. Thus, the sum over α on the right hand side of Eq. (22b) implies a divergence. But if we fix α to one single value or normalize with respect to the number of Floquet replicas considered for this purpose, one obtains a nice sum rule again

$$\sum_{m,n=0}^{\infty} (p_m \pm p_n) |F_{m,n}|^2 = \sum_m p_m \langle m, 0 | [c, c^\dagger]_{\pm} | m, 0 \rangle \quad (24a)$$

$$= \langle [c, c^\dagger]_{\pm} \rangle \Big|_{t=0} \quad (24b)$$

$$= 1, \quad (24c)$$

where the last equation holds for c a fermionic or bosonic single-particle annihilation operator.

Summarizing, we considered a broad range of nonequilibrium systems which are in the Floquet regime, i.e., they are given in a mixture of quasi-stationary Floquet states which solve the time-dependent Schrödinger equation. For this setting, we rigorously established a generalization of the Lehmann representation. The spectral representation of two-time Floquet response functions include the cases of fermionic and bosonic single-particle propagators. We clarified the relation to the Wigner representation, which exploits the periodicity in the average time of the two times and to the Floquet representation. Our results show precisely when fermionic spectral functions must be nonnegative and can be interpreted as densities-of-states. We also established some exact sum rules.

As an outlook, we think that more information on the mathematical properties of the self-energy in the Floquet regime is also desirable. In equilibrium, for instance, one deduces from the Dyson equation that the imaginary part of the self-energy is also nonnegative. Does a similar result holds in the Floquet regime? One might conjecture that the self-energy averaged over t_{ave} should also behave as in equilibrium. But the Floquet Dyson equation is too complicated and does not appear to permit one to establish this fact.

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