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An exact sum-rule for the Hubbard model: an historical approach.

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Abstract. The aim of the present article is to derive an exact integral equation for the Green function of the Hubbard model through an equation-of-motion procedure, like in the original Hubbard papers. Though our exact integral equation does not allow to solve the Hubbard model, it represents a strong constraint on its approximate solutions. An analogous sum rule has been already obtained in the literature, through the use of a spectral moment technique. We think however that our equation-of-motion procedure can be more easily related to the historical procedure of the original Hubbard papers. We also discuss examples of possible applications of the sum rule and propose and analyse a solution, fulfilling it, that can be used for a pedagogical introduction to the Mott-Hubbard metal-insulator transition.

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keywords: Hubbard model, Mott metal-insulator transition, Green functions

1. Introduction

Since its introduction in 1963 [1], the Hubbard model has been commonly used to describe strongly-correlated electron systems in narrow-energy bands. The reason is that when the Coulomb repulsion (U) is bigger than the electron bandwidth (W), the atomic-limit approach followed by Hubbard in his original papers[1, 2, 3] is justified. This approach has been found very fruitful, giving rise to several subfields of application still on fashion (more than 150 articles per year published on the subject in recent years[4]). The model owes its fame to the fact that it represents a ‘minimal’ hamiltonian to study electron correlations in crystal materials. However, in spite of its relative formal simplicity (see Eq. (1) below), the Hubbard model can be solved exactly only in one [5] and infinite [6, 7] dimensions. The behaviour of its ground-state phase diagram in the most important cases of two and three dimensions is rather deduced by approximate solutions, usually determined by the competing actions of the Coulomb electron repulsion U and of the kinetic energy of the electrons in the periodic field of the nuclei (hopping-energy, t). A general overview of the formal properties of the Hubbard model can be found in Ref. [8] and a review of several approximate solving schemes in use today can be found in Ref. [9].

However, an old-standing lesson about the Hubbard model [10] is that the model itself should not be confused with any of its approximate solutions. For example, the first approximate solution historically found (Hubbard I[1]) was known to have the drawback of being insulating for whatever value of $U \neq 0$ (even $U \ll W$), whereas, physically, one would expect a finite critical value U_c (of the order of the bandwidth W), above which the insulating solution is stabilized and below which the material is a metal (except for the one-dimensional case, see the discussion in Section III). Drawbacks like this are due to the lack of control of the approximations performed and they might be cured, at least partially, by the specification of proper constraints on the solution, as we shall see below.

Historically, the model had been attacked by Hubbard through a Green function formalism, based on the equation-of-motion approach [1, 2, 3, 11, 12, 13, 14, 15]. Within this approach a succession of coupled equations of motion for the Green functions is written down. However, the set of equations of motion turns out to be infinite so that some decoupling procedures must be introduced to simplify it. The usual decoupling procedure consists in expressing a Green function of the set in terms of another (or more). In this way, the specific decoupling procedure that is adopted determines the subsequent dynamics of the system, as it was the case for the original Hubbard I [1] and Hubbard III [3] solutions (as well as for several others during the next years [12, 13, 14, 15]). In spite of the historical importance of the equation-of-motion decoupling procedure, such an approach, as sketched above, could not guarantee a proper control on the kind of approximation performed, mainly because of the lack of exact constraints for the obtained Green functions.

The aim of the present paper is to partially fill this gap and derive an exact integral

equation for the Green function of the Hubbard model, Eq. (9) below. Mathematically, the key features allowing us to derive the exact sum rule are 1) a limiting procedure in the time domain, together with 2) the time translation invariance of all Green functions $G(t - t')$, so that their derivative with respect to t is equal to the opposite of the one with respect to t' . Unfortunately, this sum rule does not allow to recover the full Green function, but it can be used as a constraint on the approximate solutions. For example, as shown in Appendix A, we can check, among all approximated solutions proposed in the literature, like the mean-field, Hubbard I or Hubbard III solutions, which one respects the exact constraint imposed by Eq. (9) and which one should be instead discarded. An anonymous Referee remarked that two recent publications [16, 17] show that it is possible to apply the momentum sum-rules to out-of-equilibrium conditions, thereby suggesting that the constraint on time-translation invariance can be relaxed. A brief description of this idea in our case is given in Appendix B.

It should be noticed that our final result is not completely new, because the imaginary part of Eq. (9) can be found equivalent to a given linear combination of the exact sum rules for spectral momenta obtained in Ref. [18]. This is detailed at the end of Appendix A. Yet, we can highlight two original features in our result. Firstly, the solution that we propose in Section III, as detailed below, can be a useful pedagogical complement to the original approximations, allowing to highlight some of their drawbacks, like in the Mott-Hubbard metal-insulator transition. In second place, the procedure that we used to derive it is based on the same equation-of-motion approach as in the original Hubbard articles that are usually studied by PhD students. For this reason, differently from Ref. [18], our approach can be taught to young researchers in the field, in parallel to the original articles[1, 2, 3] introducing to the Hubbard model.

The plan of the paper is the following: in section II we remind the basic features of the equation-of-motion approach for the Green functions, with a direct reference to the historical Hubbard articles. We then derive our sum rule, Eq. (9), by applying the trick described above of deriving with respect to t' , instead of t . In doing this, we describe carefully the mathematical derivation of the limiting procedure for a distribution. In section III we discuss a solution compatible with the sum rule, characterized by a real-self-energy. This solution can be considered as an improvement of the Hubbard I solution, and therefore can be used in its place as a toy-model by students to investigate the non-Fermi liquid character of the solution. Finally, in Appendix A some exact mathematical implications of the sum-rule are reported. In particular, the constraint implied by Eq. (9) is applied to well-known approximate solutions of the Hubbard model (atomic limit, mean-field, Hubbard I and Hubbard III). Appendix B shows how to apply the sum rule in out-of-equilibrium conditions, following Ref. [17].

2. Derivation of the sum rule

The Hubbard Hamiltonian on a crystal lattice, in its simplest version with one orbital per site [1], can be expressed as:

$$\hat{H}_H = \sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad (1)$$

Here $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{j\sigma}$) represents, in standard notation, the creation (annihilation) of an electron of spin σ at site i (j), t_{ij} is the energy associated to the hopping from site j to site i (supposed translationally invariant) and U is the on-site Coulomb repulsion. The term $t_{ii} \equiv \varepsilon_0$ represents the local energy at site i and it can be put equal to zero without any loss of generality.

Following Ref. [19], we can define the retarded Green function: $i\hbar G_{ij\sigma}^{(R)}(t-t') \equiv \theta(t-t') \langle \{ \hat{c}_{i\sigma}(t), \hat{c}_{j\sigma}^\dagger(t') \} \rangle$, by introducing the Heaviside function $\theta(t-t') = 1$ if $t \geq t'$ and 0 if $t < t'$. The $\{ \dots, \dots \}$ represents the anticommutator of the fermion operators. We have chosen the retarded Green function in keeping with the original Hubbard articles [1, 2, 3]. However, all what is reported below is equally valid for the advanced Green function, $i\hbar G_{ij\sigma}^{(A)}(t-t') \equiv -\theta(t'-t) \langle \{ \hat{c}_{i\sigma}(t), \hat{c}_{j\sigma}^\dagger(t') \} \rangle$, and the time-ordered Green function, $i\hbar G_{ij\sigma}^{(T)}(t-t') \equiv \theta(t-t') \langle \hat{c}_{i\sigma}(t) \hat{c}_{j\sigma}^\dagger(t') \rangle - \theta(t'-t) \langle \hat{c}_{j\sigma}^\dagger(t') \hat{c}_{i\sigma}(t) \rangle$. We remark, however, that it is not valid for two other Green functions often in use [20], the greater, $i\hbar G_{ij\sigma}^>(t-t') \equiv \langle \hat{c}_{i\sigma}(t) \hat{c}_{j\sigma}^\dagger(t') \rangle$, and the lesser, $i\hbar G_{ij\sigma}^<(t-t') \equiv -\langle \hat{c}_{j\sigma}^\dagger(t') \hat{c}_{i\sigma}(t) \rangle$, whose analytical properties are different [17], in particular they lack the time-discontinuity leading to the delta-function in their derivative, as in Eq. (2) below.

All expectation values can be calculated either at $T = 0$ or, for finite temperature, through the grand-canonical statistical weight, $e^{-\beta(\hat{H}_H - \mu \hat{N})}$, where \hat{N} is the number operator and μ the chemical potential, as in [19].

If we write the equation of motion of the Green function in the time-domain, instead of the frequency (ω)-domain as in Hubbard papers, we get (we omit the label (R) in what follows):

$$i\hbar \partial_t G_{ij\sigma}(t-t') = i\hbar \delta_{ij} \delta(t-t') - \mu G_{ij\sigma}(t-t') + \sum_l t_{il} G_{lj\sigma}(t-t') + U \Gamma_{ij\sigma}(t-t') \quad (2)$$

where $\Gamma_{ij\sigma}(t-t') \equiv \theta(t-t') \langle \{ \hat{n}_{i\bar{\sigma}}(t) \hat{c}_{i\sigma}(t), \hat{c}_{j\sigma}^\dagger(t') \} \rangle$.

Here we have used the Heisenberg formula for the time-derivation of Heisenberg operators: $i\hbar \partial_t \hat{c}_{i\sigma}(t) = [\hat{c}_{i\sigma}(t), \hat{H}_H]$, where $[\dots, \dots]$ represents a commutator. We remind that all the creation and annihilation operators in the Green functions defined above are taken in the Heisenberg representation [19], i.e., their time-evolution is governed by the full Hamiltonian H_H . We also used the well-known relation, valid for distributions: $\partial_t \theta(t-t') = \delta(t-t')$.

In the original Hubbard article and in all the subsequent developments [1, 2, 3, 11, 12, 13, 14, 15], the chain of equations of motion is continued by deriving $\Gamma_{ij\sigma}(t-t')$ with respect to t [21]. However, by using the time-translational invariance of the Green functions due to the dependence on the time-difference ($t-t'$), we can instead derive with respect to t' and write, after Eq. (2):

$$\begin{aligned}
 i\hbar\partial_t\Gamma_{ij\sigma}(t-t') &= -i\hbar\partial_{t'}\Gamma_{ij\sigma}(t-t') = \delta_{ij}n_{i\bar{\sigma}}\delta(t-t') - \mu\Gamma_{ij\sigma}(t-t') \\
 &\quad + \sum_l t_{il}\Gamma_{lj\sigma}(t-t') + UM_{ij\sigma}(t-t') \quad (3)
 \end{aligned}$$

The main difference with the Hubbard original approach is that the hopping term on the right-hand side of Eq. (3) does not lead to a new set of functions as in the usual chain [1, 3], but to the same function $\sum_l t_{il}\Gamma_{lj\sigma}(t-t')$, that can be easily diagonalised by a Fourier transform. This time, the unknown is the new Green function $M_{ij\sigma}^{(R)}(t-t') \equiv \theta(t-t')\langle\{\hat{n}_{i\bar{\sigma}}(t)\hat{c}_{i\sigma}(t), \hat{n}_{j\bar{\sigma}}(t')\hat{c}_{j\sigma}^\dagger(t')\}\rangle$ (for the retarded case). Of course writing down the equation of motion for $M_{ij\sigma}(t-t')$ would continue the infinite set in a different way from the usual one. This would lead to an infinite set of exact relations amongst higher-order Green functions, that can be left as an exercise to the interested reader.

We shall however proceed differently. In order to derive the sum rule for $G_{ij\sigma}(t-t')$, we notice that it is possible to find a point in space-time where $M_{ij\sigma}(t-t') = \Gamma_{ij\sigma}(t-t')$ exactly: this happens for $i = j$ and $t - t' \rightarrow 0^\pm$. Mathematically, we have, for the retarded Green function:

$$\begin{aligned}
 \lim_{t-t'\rightarrow 0^+} M_{ii\sigma}(t-t') &= \langle\{\hat{n}_{i\bar{\sigma}}(t)\hat{c}_{i\sigma}(t), \hat{n}_{i\bar{\sigma}}(t)\hat{c}_{i\sigma}^\dagger(t)\}\rangle = \langle\{\hat{n}_{i\bar{\sigma}}(t)\hat{n}_{i\bar{\sigma}}(t)\hat{c}_{i\sigma}(t), \hat{c}_{i\sigma}^\dagger(t)\}\rangle \\
 &= \langle\{\hat{n}_{i\bar{\sigma}}(t)\hat{c}_{i\sigma}(t), \hat{c}_{i\sigma}^\dagger(t)\}\rangle = \lim_{t-t'\rightarrow 0^+} \Gamma_{ii\sigma}(t-t') \quad (4)
 \end{aligned}$$

In the second equality of the equation, we have used the commutativity at equal times of $\hat{n}_{i\bar{\sigma}}(t)$ and $\hat{c}_{i\sigma}(t)$ or $\hat{c}_{i\sigma}^\dagger(t)$ (opposite spin) and in the third equality the projection property of the number operator $\hat{n}_{i\bar{\sigma}} = \hat{n}_{i\bar{\sigma}}^2$. A similar derivation can be easily derived for the advanced and time-ordered Green functions as well.

Physically, this property is easily understandable: $M_{ij\sigma}(t-t')$ represents the probability that an electron (or a hole), created at site j at time t' (making the site j doubly occupied) is destroyed at a site i that is also doubly occupied at time t . Instead, $\Gamma_{ij\sigma}(t-t')$ represents the probability that an electron (or a hole), created at site j at time t' (making site j either singly or doubly occupied) is destroyed at time t at a site i that is (again) doubly occupied. Clearly, if $i = j$ and $t - t' \rightarrow 0^\pm$, we are dealing with the same site at the same time. So, if this site is doubly occupied for the destruction process, it must be made doubly occupied by the creation process, thereby leading to the equality of the two Green functions, Γ and M .

By inserting Eq. (4) into Eq. (3), by taking $i = j$ and performing the $\lim_{t-t'\rightarrow 0^+}$ of both the left-hand-side and the right-hand-side, we can derive the sum rule. The safest way to handle the limit procedure on distributions, like the delta function, characterized by a discontinuity at $t = t'$, is to move to the Fourier transform first, and then perform the $\lim_{t-t'\rightarrow 0^+}$ by keeping track of the convergence factor $e^{-(t-t')\eta}$. In fact, as shown,

e.g., in Ref. [19], the time-frequency ($t \leftrightarrow \omega$) Fourier transform of Green functions is not properly defined unless a convergence factor $e^{\pm(t-t')\eta^+}$ is introduced, where η is a small imaginary part of the frequency and $\eta \rightarrow 0$ at the end of the calculation. For G^R , η is a small positive quantity forcing the displacement of the poles in the complex- ω plane out of the real ω axis, thereby allowing the integrability of the Fourier transform[19]. We notice here that the advanced and time-ordered Green functions have a different analytical structure than the retarded one (η has the opposite sign for $G^{(A)}$ and the opposite sign below the chemical potential for $G^{(T)}$, see [19]). However, an analogous sum-rule can be written for these two Green functions as well. With this in mind, we can continue from equation (3) with $i = j$:

$$\begin{aligned} \lim_{t-t' \rightarrow 0^+} \left(i\hbar \partial_t \int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} \Gamma_{\vec{k}\sigma}(\omega) e^{-i[\omega(t-t')]} \right) &= \lim_{t-t' \rightarrow 0^+} n_{i\bar{\sigma}} \int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} e^{-i[\omega(t-t')]} \\ &+ \lim_{t-t' \rightarrow 0^+} \left((U - \mu) \int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} \Gamma_{\vec{k}\sigma}(\omega) e^{-i[\omega(t-t')]} \right. \\ &\left. + \sum_l t_{il} \int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} \Gamma_{\vec{k}\sigma}(\omega) e^{-i[\omega(t-t') - \vec{k} \cdot (\vec{R}_l - \vec{R}_i)]} \right) \quad (5) \end{aligned}$$

where \vec{k} -integrals are extended over the Brillouin zone, ω -integrals from $-\infty$ to $+\infty$ and s represents the dimensionality of the system (the present derivation is valid for any dimensions). We notice that $n_{i\bar{\sigma}}$ appearing in Eq. (5) is no more an operator, but a number: it is the expectation value $n_{i\bar{\sigma}} \equiv \langle \hat{n}_{i\bar{\sigma}} \rangle$. If we first perform the time-derivative of the left-hand-side and then the limit of both sides, we obtain an integral expression for $\Gamma_{\vec{k}\sigma}(\omega)$:

$$\int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} [(\hbar\omega + \mu - t_{\vec{k}} - U)\Gamma_{\vec{k}\sigma}(\omega) - n_{\bar{\sigma}}] = 0 \quad (6)$$

where we have supposed an homogeneous system, so that $n_{i\bar{\sigma}} = n_{\bar{\sigma}}$. This position excludes the possibility of antiferromagnetic solutions (we refer to, e.g., [22] for an explicit antiferromagnetic calculation with inhomogeneous $n_{i\bar{\sigma}}$, for the simpler mean-field solution of the Hubbard model). We can now Fourier transform the equation (2) for the Green function:

$$(\hbar\omega + \mu - t_{\vec{k}})G_{\vec{k}\sigma}(\omega) = 1 + U\Gamma_{\vec{k}\sigma}(\omega) \quad (7)$$

solve for $\Gamma_{\vec{k}\sigma}(\omega)$:

$$\Gamma_{\vec{k}\sigma}(\omega) = \frac{1}{U}(\hbar\omega + \mu - t_{\vec{k}})G_{\vec{k}\sigma}(\omega) - \frac{1}{U} \quad (8)$$

and replace in (6):

$$\int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} [(\hbar\omega + \mu - t_{\vec{k}} - U)(\hbar\omega + \mu - t_{\vec{k}})G_{\vec{k}\sigma}^-(\omega) - (\hbar\omega + \mu - t_{\vec{k}} - U(1 - n_{\bar{\sigma}}))] = 0 \quad (9)$$

This is the main result of our work, an exact integral equation for $G_{\vec{k}\sigma}^-(\omega)$, to be used with the appropriate boundary conditions. Though it does not allow for a full determination of the Green function, our integral equation acts as a constraint that must be fulfilled by the exact solution. We remind again that, in order to derive it, we used the following two ingredients: (a) contrary to what is done in the Hubbard papers and in the literature, we have written the equation of motion of $\Gamma(t - t')$ with respect to t' instead of t . Using the translational invariance of any Green function due to the dependence on $(t - t')$, we have $\partial_t \Gamma_{ij\sigma}(t - t') = -\partial_{t'} \Gamma_{ij\sigma}(t - t')$; (b) we performed a limit procedure in the time-domain for the on-site Green functions $M_{ii\sigma}(t - t')$ and $\Gamma_{ii\sigma}(t - t')$.

From now on, to simplify notations, we shall measure the energy from the chemical potential, thereby replacing $t_{\vec{k}} - \mu$ with $t_{\vec{k}}$.

3. Discussion.

Among all possible solutions of Eq. (9), the simplest one is obtained by imposing the integrand function equal to zero. This implies, e.g., for the retarded Green function:

$$G_{\vec{k}\sigma}^R(\omega) = \frac{1 - n_{\bar{\sigma}}}{\hbar\omega - t_{\vec{k}} + i\eta} + \frac{n_{\bar{\sigma}}}{\hbar\omega - t_{\vec{k}} - U + i\eta} \quad (10)$$

Equation (10) represents a two-pole Green-function with real self-energy (infinite time-life of the two quasiparticles). The self-energy $\Sigma_{\vec{k}}(\omega)$ associated to this solution can be obtained from its definition: $G_{\vec{k}\sigma}^R(\omega) = [\hbar\omega - t_{\vec{k}} - \Sigma_{\vec{k}}(\omega) + i\eta]^{-1}$. By comparing the latter to Eq. (10), we obtain: $\Sigma_{\vec{k}}(\omega) = U \frac{(\hbar\omega - t_{\vec{k}})n_{\bar{\sigma}}}{\hbar\omega - t_{\vec{k}} - U(1 - n_{\bar{\sigma}})}$.

Such a solution represents non-mixing Hubbard quasiparticles, i.e., electrons moving in a singly occupied band and electrons moving in a doubly occupied band, respectively, without intercrossing. Equation (10) is in fact the solution that we would have obtained from Eq. (3) by putting $M_{ij} = \Gamma_{ij}$ identically. This corresponds to approximating the two probabilities P_M and P_Γ , where P_M is the probability that an electron is created at a site making it doubly-occupied and then decays at another doubly occupied site. Instead P_Γ is the probability that an electron created at a site with any filling decays at a doubly occupied site. These processes are depicted in Fig. 1. Such an approximation becomes true in the limit where $n_{\bar{\sigma}} = 1$: in this case any σ -electron would fall on a singly-occupied site, making it doubly occupied. The behaviour of the density of states $\rho_\sigma(\varepsilon)$, in the specific case of a square-lattice band, $t_{\vec{k}} = 2t[\cos(k_x a) + \cos(k_y a)]$, with a the lattice unit, is represented in Fig. 2, and is given by the equation: $\rho_\sigma(\varepsilon) = \frac{1}{N} \sum_{\vec{k}} \left\{ (1 - n_{\bar{\sigma}}) \delta \left[\varepsilon - \varepsilon_{\vec{k}}^{\text{LHB}} \right] + n_{\bar{\sigma}} \delta \left[\varepsilon - \varepsilon_{\vec{k}}^{\text{UHB}} \right] \right\}$. Here

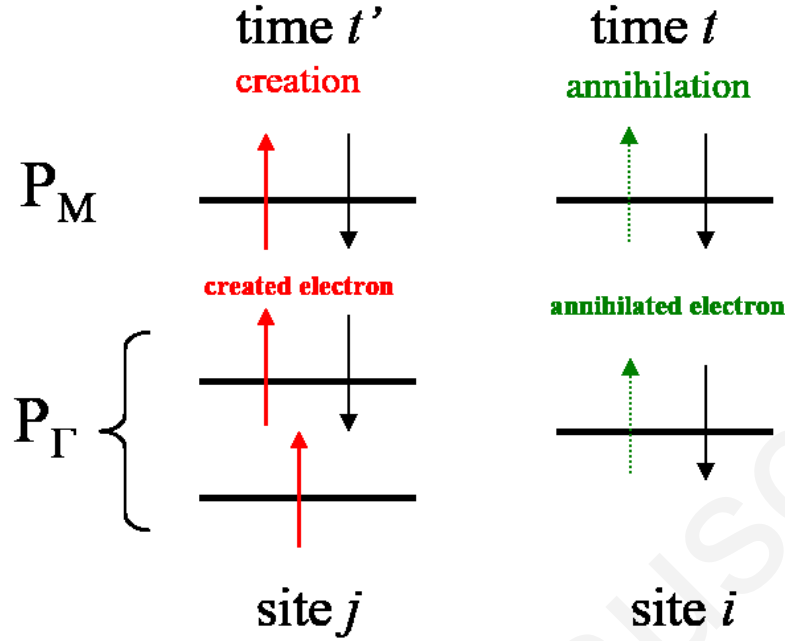


Figure 1. Visualization of the probabilities P_M and P_Γ described in the text. In (a), P_M , an electron \uparrow is created at site j , already occupied by an electron \downarrow . Instead, in (c), P_Γ , an electron \uparrow is created at site j independently of its occupancy. The annihilation process is the same for both P_M and P_Γ : the electron is annihilated from a doubly-occupied site i , as in (b) and (d).

$\varepsilon_{\vec{k}}^{\text{LHB}} = t_{\vec{k}}$ and $\varepsilon_{\vec{k}}^{\text{UHB}} = t_{\vec{k}} + U$ are the lower Hubbard band and the upper Hubbard band, respectively, as deduced from the imaginary part of Eq. (10) [22].

As shown in Fig. 2(a), at half-filling, i.e., when $n_\sigma = n_{\bar{\sigma}} = 0.5$, the Fermi energy is within the gap and the system is a Mott insulator when U/t is above a critical value $(U/t)_c = 8$ (or $(U/W)_c = 1$, as the bandwidth W , for a 2D square lattice, is $W = 8t$). If instead U/W is below the critical value, the two bands merge and the system behaves like a metal (this is shown in Fig. 2(a) for the value $U/W = 3/8$). It is useful to remind that, even in the metallic state, an important feature of the atomic behaviour is still present: each \vec{k} point has a spectral weight $(1 - n_{\bar{\sigma}})$ in the LHB and $n_{\bar{\sigma}}$ in the UHB, differently to the one-to-one correspondence of a Fermi-liquid behaviour. So, even in the metallic state, the solution (10) does not represent a ‘normal’ metal, i.e., a Fermi liquid. In fact, it does not fulfill the Luttinger’s theorem [23], which necessarily characterizes Fermi liquids when the interaction is adiabatically switched on from the Fermi gas. It is interesting to notice that, though at a qualitative level the Hubbard model is often described to have these features, we could not find any derivation of Eq. (10) in the literature through the approximation $M_{ij} = \Gamma_{ij}$.

Equation (10), having a real self-energy leads to an infinite lifetime for the two sub-bands quasiparticles, analogously to the Hubbard I solution. However, Eq. (10)

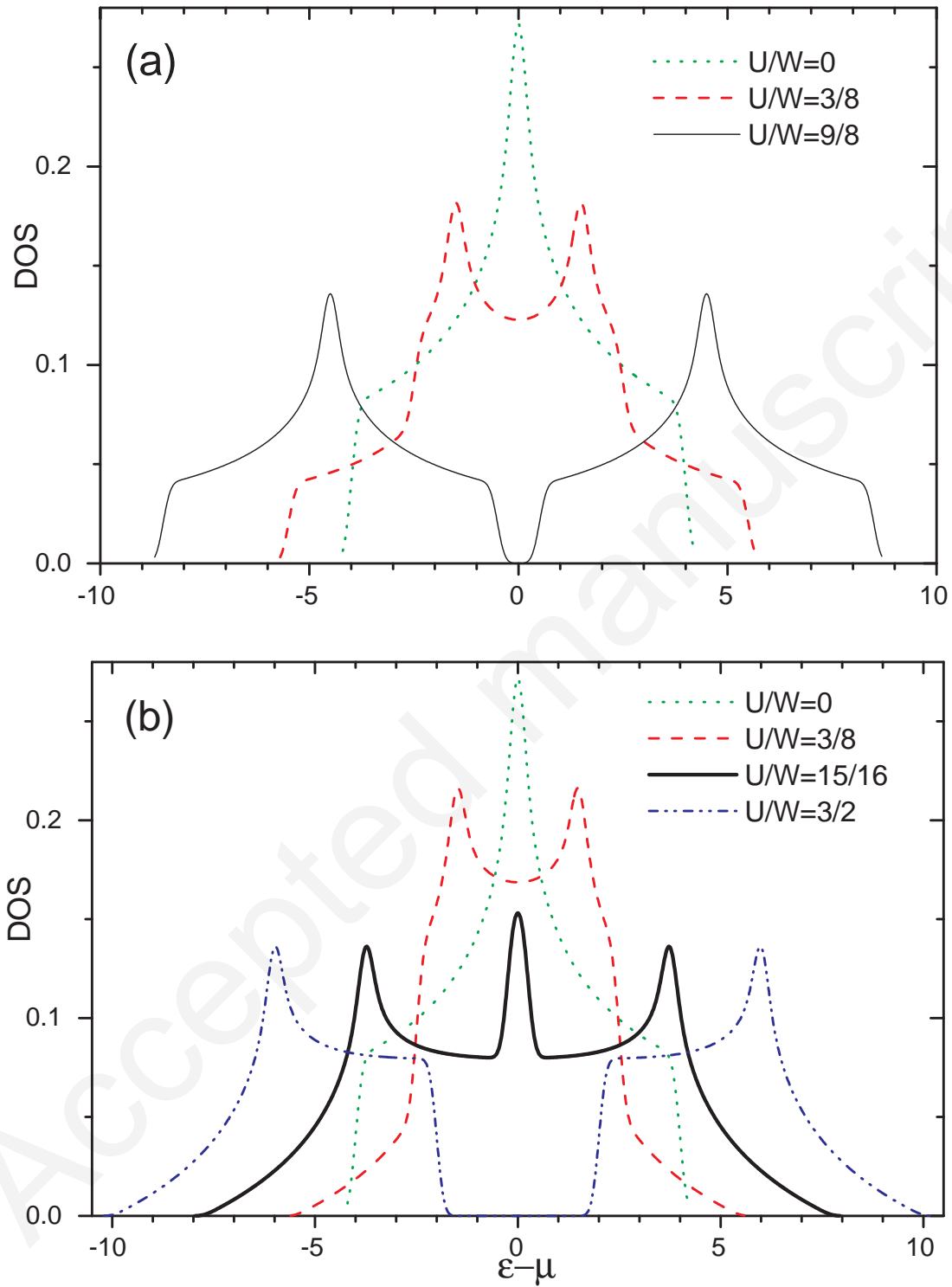


Figure 2. Density of states at half-filling ($n_\sigma = n_{\bar{\sigma}} = 0.5$) corresponding to: (a) Eq. (10); (b) Eq. (11). The Mott-Hubbard metal-insulator transition is present for $U/W \sim 1$ in both cases. The extra peak shown in (b) around the Fermi energy ($\epsilon = \mu$) is not of dynamical origin (see main text for further remarks).

has the advantage of not suffering from the same drawbacks as the Hubbard I solution, because it respects our sum-rule Eq. (9). In particular, contrary to the Hubbard I metal-insulator transition, found even for an infinitesimal value of U/W , which is unphysical in more than one spatial dimensions, our solution more realistically gives $U/W \sim 1$.

An interesting, different, behaviour appears when we consider a solution of Eq. (9) more general than Eq. (10):

$$G_{k\sigma}^R(\omega) = \frac{1 - n_{\bar{\sigma}} + g_{\vec{k}}(\omega)}{\hbar\omega - t_{\vec{k}} + i\eta} + \frac{n_{\bar{\sigma}} - g_{\vec{k}}(\omega)}{\hbar\omega - t_{\vec{k}} - U + i\eta} \quad (11)$$

where $g_{\vec{k}}(\omega)$ is not determined by Eq. (9) except for having a null integral in the Brillouin zone:

$$\int \frac{d^s \vec{k}}{(2\pi)^s} g_{\vec{k}}(\omega) = 0 \quad (12)$$

The self-energy associated to this solution is: $\Sigma_{\vec{k}}(\omega) = U \frac{(\hbar\omega - t_{\vec{k}})(n_{\bar{\sigma}} - g_{\vec{k}}(\omega))}{\hbar\omega - t_{\vec{k}} - U(1 - n_{\bar{\sigma}} + g_{\vec{k}}(\omega))}$. In this case, provided that Eq. (12) is fulfilled, the function $g_{\vec{k}}$ can be ω -dependent. We remark that, in spite of the ω -dependent self-energy, the density of states obtained from $\Sigma_{\vec{k}}(\omega)$ has a two-pole structure (as derivable also from the imaginary part of Eq. (11)), with ω -dependent spectral weight, so as to have spectral-weight transfer within the two bands, but not damping. This can be seen if we write the retarded Green function as: $G_{k\sigma}^R(\omega) = [\hbar\omega - t_{\vec{k}} - \Sigma_{\vec{k}}(\omega) + i\eta]^{-1}$. In this case the density of states is: $\rho_{\sigma}(\varepsilon) = -\frac{\pi}{N} \sum_{\vec{k}} \Im G_{k\sigma}^R(\omega) = \frac{1}{N} \sum_{\vec{k}} \delta[\varepsilon - t_{\vec{k}} - \Sigma_{\vec{k}}(\omega)]$. This expression can be written as: $\rho_{\sigma}(\varepsilon) = \frac{1}{N} \sum_{\vec{k}} \delta \left[\frac{(\varepsilon - t_{\vec{k}})(\varepsilon - t_{\vec{k}} - U)}{\varepsilon - t_{\vec{k}} - U(1 - n_{\bar{\sigma}} + g_{\vec{k}}(\omega))} \right]$. By reminding that $\delta(h(x)) = \sum_i \delta(x - x_i)/h'(x_i)$, where x_i are the zeros of $h(x)$, it is easy to derive, from the previous expression, that $\rho_{\sigma}(\varepsilon) = \frac{1}{N} \sum_{\vec{k}} \left\{ (1 - n_{\bar{\sigma}} + g_{\vec{k}}(\omega)) \delta[\varepsilon - t_{\vec{k}}] + (n_{\bar{\sigma}} - g_{\vec{k}}(\omega)) \delta[\varepsilon - t_{\vec{k}} - U] \right\}$.

We might have a hint for $g_{\vec{k}}$, limiting to a ω -independent form, on the basis of the following concept. If we consider a frozen configuration (no hopping, $t = 0$), the probability that a spin- σ electron put randomly in the lattice falls on an unoccupied site (so as to give single occupancy) is proportional to $1 - n_{\bar{\sigma}}$ and the probability that it falls on a $\bar{\sigma}$ -occupied site (so as to give double occupancy) is proportional to $n_{\bar{\sigma}}$. This corresponds to the two numerators of Eq. (11) when $g_{\vec{k}}(\omega) = 0$. However, when $t \neq 0$, the hopping changes these assignments, by allowing intersite motion. The changes in the spectral weights (numerators) of Eq. (11) determined by the function $g_{\vec{k}}(\omega)$ are a measure of this motion. If we suppose, as it appears plausible, that this motion is proportional to both the filling $n_{\bar{\sigma}}$ and the hopping $t_{\vec{k}}$ then a possible form for $g_{\vec{k}}(\omega)$, independent of ω , is $g_{\vec{k}} = n_{\bar{\sigma}} t_{\vec{k}}/W$, that satisfies condition (12). At half-filling, we obtain the density of states represented in Fig. 2(b), as a function of the ratio U/W . Compared to Fig. 2(a), there is a shift in spectral weight from the UHB to the LHB (and vice-versa), around the Fermi energy ($\varepsilon = \mu$) close to the metal-to-insulator transition. For $U/W = 15/16$, this shift in spectral weight gives rise to an extra peak in the density

of states at the Fermi energy, leading to a strong increase in all the physical properties (like the specific heat, Pauli paramagnetism or the electric conductivity) that linearly depend on $\rho(\mu)$, the value of the density of states at the Fermi energy. Interestingly, a peak in the density of states at the Fermi energy close to a metal-insulator transition is usually considered a signature of a ‘strange-metal’ behaviour [24]. However, in this case, the origin of this peak is not dynamical, as we have neglected the ω -dependence of $g_{\vec{k}}$: its origin is rather due to a \vec{k} -redistribution of the spectral weight determined by the function $g_{\vec{k}}$. So, it does not share the same origin as the central peak in the density of states of dynamical mean-field theory [24, 6]. We remark that neither our approximate solution Eq. (10) nor Eq. (11) describes correctly the one-dimensional limit. In fact, both Eqs. (10) and (11) provide the uncorrect result $(U/W)_c \sim 1$ even in this limit, instead of the correct one-dimensional result, $(U/W)_c = 0$.

We would like to end this section by moving from an academic approach to actual research, and highlight that our real self-energy solution, Eq. (10) shows an interesting complementarity with the well-known LDA+U method [25, 26] in density-functional theory. The latter is a multiorbital unrestricted mean-field approach that advantages orbital (and charge) separation, compared to a bare LDA calculation, because of the U -term: once the average Coulomb energy is subtracted from a LDA calculation, an energy shift U is attributed, compared to the LDA band $t_{\vec{k}}$, to doubly occupied orbitals so as to reduce the fractional occupancy of these orbitals in favour of an integer one. This can force the system towards an insulating state but, in order to do that, a multiband material is needed, because the U energy shift is obtained only for doubly-occupied orbital bands relatively to singly-occupied orbital bands. The latter is the main difference with our approach: with Eq. (10) a metal-insulator transition is possible within just one orbital band, as shown in Fig. 2: this is a consequence of the loss of validity of Luttinger’s theorem (not shared by the LDA+U approach), leading to two different quasiparticle species for a given \vec{k} . It is the splitting of the single-orbital band in two subbands (as shown in Fig. 2) that makes the difference with the LDA+U method (where there is no splitting for a single band). In order to perform a more complete comparison of the two approaches, our solution should be extended to the multiorbital case. However, this would go beyond the scope of a pedagogical presentation and will rather be the object of a future research work.

4. Conclusions

In conclusions, we have derived in Section II an exact sum rule (Eq. (9)) for the Green function of the Hubbard model, and we have discussed in Section III a solution of the model satisfying this sum rule. Previous solutions not respecting this constraint have been highlighted. The derivation has been performed with an approach and a detail of particulars that should be convenient to PhD students working in the field. The aim is to use the proposed solution for the Green function, Eq. (10), as an alternative to the first Hubbard solution (Hubbard I), without the drawbacks of the latter.

Besides the pure academic scope, the interest of Eq. (11) with respect to actual research work is also highlighted in the last part of Section III.

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Appendix A. Comparison of Eq. (9) with previous results

In this Appendix, we show how our exact result, Eq. (9), can be used to highlight some weaknesses of the historical approximations Hubbard I [1] and Hubbard III [3]. However, as a first check, it is possible to verify that Eq. (9) is satisfied both in the atomic limit, i.e., when $t_{\vec{k}} \rightarrow \varepsilon_0$ (ε_0 is the atomic on-site energy) and in the band limit, i.e., when $U = 0$. In the first case, considering for example the retarded Green function, we get $G_{\text{at},\sigma}^{(R)}(\omega) = (1 - n_{\bar{\sigma}})/(\hbar\omega - \varepsilon_0 + i\eta) + n_{\bar{\sigma}}/(\hbar\omega - \varepsilon_0 - U + i\eta)$ and in the second case $G_{0\vec{k}\sigma}^{(R)}(\omega) = 1/(\hbar\omega - t_{\vec{k}} + i\eta)$. Both satisfy Eq. (9), as can be seen by direct inspection. Even if we consider the non-local correlations that should be present in a proper atomic limit for $G_{\text{at},\sigma}^{(R)}(\omega)$ (see section IV of Ref. [12]), Eq. (9) is still satisfied. The equation is however not satisfied by the mean-field Green function and the Hubbard I and Hubbard III Green functions. In fact, if we replace in Eq. (9) the mean-field retarded Green function $G_{\vec{k}\sigma}^{(R)}(\omega) = 1/(\hbar\omega - t_{\vec{k}} - Un_{\bar{\sigma}} + i\eta)$, we get the result $i\pi U^2 n_{\bar{\sigma}}(1 - n_{\bar{\sigma}})$ instead of zero. The calculation is performed by reminding that $(x + i\eta)^{-1} = Px^{-1} - i\pi\delta(x)$, where P is the integral principal part and δ is the Dirac distribution. Therefore, though the integral of the real, principal part is zero, there remains a contribution from the imaginary term, showing that the spectral function of the mean-field solution (proportional to $\Im G^{(R)}$) is not correct (it does not satisfy the sum-rule Eq. (9)), unless $n_{\bar{\sigma}} = 0$ (free particles) or $n_{\bar{\sigma}} = 1$.

A slightly more complex calculation, because of the \vec{k} -dependence, shows that neither the Hubbard I nor the Hubbard III Green functions satisfy Eq. (9) (or Eq. (A.1)). In the case of Hubbard I solution, the Green function is: $G_{\vec{k}\sigma}^{(R)}(\omega) = \frac{A_{\vec{k}}^-}{\hbar\omega - E_{\vec{k}}^- + i\eta} + \frac{A_{\vec{k}}^+}{\hbar\omega - E_{\vec{k}}^+ + i\eta}$, where $E_{\vec{k}}^{\pm} = (U + t_{\vec{k}} \pm \sqrt{(U - t_{\vec{k}})^2 + 4Ut_{\vec{k}}n_{\bar{\sigma}}})/2$ is the energy spectrum and $A_{\vec{k}}^{\pm} = (E_{\vec{k}}^{\pm} - U(1 - n_{\bar{\sigma}}))/(E_{\vec{k}}^{\pm} - E_{\vec{k}}^{\mp})$ are the spectral weights. Replacement of this Green function in Eq. (9) gives again a non-zero imaginary part, that, in the simplifying case $n_{\bar{\sigma}} = 1$, is given by $i\pi(\frac{U^2}{2} + \int \frac{d^s \vec{k}}{(2\pi)^s} \frac{t_{\vec{k}}^2}{2}) \neq 0$.

Finally, in the case of the Hubbard III solution, the analysis is more complex because an explicit expression for the Green function is not available, as $G_{\vec{k}\sigma}(\omega)$ in this case is determined by means of a self-consistent calculation on five equations (Eqs. (57) to (61) in Ref. [3]). However, it is possible in this case to compare the limiting behaviour for $\omega \rightarrow \infty$ of the Hubbard III self-energy with a modified form of Eq. (9). In fact, if we write the Green function in terms of its self-energy $\Sigma_{\vec{k}\sigma}(\omega)$ as $G_{\vec{k}\sigma}(\omega) = 1/(\hbar\omega - t_{\vec{k}} - \Sigma_{\vec{k}\sigma}(\omega))$, then we can rewrite Eq. (9) as a constraint on the

self-energy as:

$$\int \frac{d^s \vec{k}}{(2\pi)^s} \int \frac{d\omega}{2\pi} \frac{[(\Sigma_{\vec{k}\sigma}(\omega) - Un_{\bar{\sigma}})\hbar\omega - \Sigma_{\vec{k}\sigma}(\omega)(t_{\vec{k}} + U(1 - n_{\bar{\sigma}})) + t_{\vec{k}}Un_{\bar{\sigma}}]}{\hbar\omega - t_{\vec{k}} - \Sigma_{\vec{k}\sigma}(\omega)} = 0 \quad (\text{A.1})$$

It should be remembered that, as from the general theory of Green functions [19] $\lim_{\omega \rightarrow \infty} G_{\vec{k}\sigma}(\omega) = 1/(\hbar\omega)$, then it follows that $\lim_{\omega \rightarrow \infty} \Sigma_{\vec{k}\sigma}(\omega)$ is a constant. Such a constant can be determined from Eq. (A.1), as in order to have a finite integral, it implies that in the limit $\omega \rightarrow \infty$ the coefficient of $\hbar\omega$ at the numerator must be zero. This gives the following constraint on the self-energy: $\lim_{\omega \rightarrow \infty} \Sigma_{\vec{k}\sigma}(\omega) = a_{\vec{k}}Un_{\bar{\sigma}} + b_{\vec{k}}$, where $\int \frac{d^s \vec{k}}{(2\pi)^s} a_{\vec{k}} = 1$ and $\int \frac{d^s \vec{k}}{(2\pi)^s} b_{\vec{k}} = 0$. This constraint is not fulfilled in the Hubbard III solution: in the notation of Ref. [3] the self-energy is $\Sigma_{\vec{k}\sigma}(E) = E - F^\sigma(E)$, with $E = \hbar\omega$, the energy, and $F^\sigma(E)$ is given by Eq. (59) of Ref. [3]. The previous constraint is fulfilled if $\lim_{E \rightarrow \infty} F^\sigma(E) = E - Un_{\bar{\sigma}}$ is true, and a direct calculation from Eq. (59) of Ref. [3] (we remind that Hubbard U was called I by Hubbard) shows that this is not the case. Interestingly, if we suppose the self-energy \vec{k} -independent, as in the case of DMFT [6], then $\lim_{\omega \rightarrow \infty} \Sigma_\sigma(\omega) = Un_{\bar{\sigma}}$, ie, dynamical mean-field exactly reduces to static mean-field in the infinite-frequency limit, as it should [27]. It is important to remind that having the correct limit for the high-energy region allows reproducing the right behaviour for the formation of the upper and lower Hubbard bands, as shown in [27], so that the former constraint, though usually neglected, should always be verified in DMFT calculations.

We finish this section by reminding that the imaginary part of Eq. (9) is equivalent to a linear combination of three sum rules for the first three momenta of the spectral function (zeroth-, first- and second-momentum sum rule). However, our full Eq. (9) (real + imaginary parts) is not just a special case of the zeroth-, first- and second-momentum sum rule, because their knowledge does not allow to derive the real part by means of Kramers-Kronig transformations, as in this case the imaginary part over the whole frequency range is needed and not just its zeroth-, first- and second-momentum. We report below an explicit calculation of the above statement, by taking, e.g. the zeroth-, first- and second-momentum sum rules of the spectral function from Ref. [28]. Setting $\Im G_{\vec{k}\sigma}^{(R)}(\omega) = -\pi S_{\vec{k}\sigma}(\omega)$, where $S_{\vec{k}\sigma}(\omega)$ is the spectral function, we can write the three sum rules as: $\int_0^{+\infty} d\omega S_{\vec{k}\sigma}(\omega) = 1$; $\int_0^{+\infty} d\omega \omega S_{\vec{k}\sigma}(\omega) = t_{\vec{k}} + Un_{\bar{\sigma}}/2$ and $\int_0^{+\infty} d\omega \omega^2 S_{\vec{k}\sigma}(\omega) = t_{\vec{k}}^2 + t_{\vec{k}}Un_{\bar{\sigma}} + U^2n_{\bar{\sigma}}/2$. If we take the imaginary part of Eq. (9), we get (we put here $\hbar = 1$): $\int d^s \vec{k} \int d\omega [(\omega - t_{\vec{k}} - U)(\omega - t_{\vec{k}})] S_{\vec{k}\sigma}(\omega) = 0$. This ω -integral can be written as: $\int d\omega \omega^2 S_{\vec{k}\sigma}(\omega) - (2t_{\vec{k}} + U) \int d\omega \omega S_{\vec{k}\sigma}(\omega) + t_{\vec{k}}(t_{\vec{k}} + U) \int d\omega S_{\vec{k}\sigma}(\omega)$. By replacing the above three sum rules in the latter expression, we get: $t_{\vec{k}}^2 + t_{\vec{k}}Un_{\bar{\sigma}} + U^2n_{\bar{\sigma}}/2 - (2t_{\vec{k}} + U)(t_{\vec{k}} + Un_{\bar{\sigma}}/2) + t_{\vec{k}}^2 + t_{\vec{k}}U$, which is identically zero, thereby showing that the imaginary part of Eq. (9) is equivalent to the above linear combination of the three sum-rules.

Appendix B. Generalization to non-equilibrium conditions.

The aim of this Appendix is to briefly show how the constraint on the time-translation invariance might be relaxed, as remarkably suggested by an anonymous Referee. We follow the idea and the notation of [17], where it is shown that the momentum sum-rules for the Hubbard model can be extended to nonequilibrium conditions, and rewrite the arguments of the Green function as t_1 and t_2 : $i\hbar G_{ij\sigma}^{(R)}(t_1, t_2) \equiv \theta(t_1 - t_2) \langle \{ \hat{c}_{i\sigma}(t_1), \hat{c}_{j\sigma}^\dagger(t_2) \} \rangle$. We do not suppose time-translation invariance. Yet, as in [17], we can define the two new variables: average time, $T = (t_1 + t_2)/2$ and relative time $t = t_1 - t_2$. The Green function depends on both of them: $i\hbar G_{ij\sigma}^{(R)}(T, t) \equiv \theta(t) \langle \{ \hat{c}_{i\sigma}(T + t/2), \hat{c}_{j\sigma}^\dagger(T - t/2) \} \rangle$, where we used the inverse transformations: $t_2 = T - t/2$ and $t_1 = T + t/2$. Because of the opposite t -dependence of t_1 and t_2 , if we derive $G_{ij\sigma}^{(R)}(t_1, t_2)$ with respect to t_1 and t_2 with the constraint of a fixed value of T (say, T_0), we get:

$$\frac{\partial G_{ij\sigma}^{(R)}(t_1, t_2)}{\partial t_2} = \frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial T} - \frac{1}{2} \frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial t} = -\frac{1}{2} \frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial t} \quad (\text{B.1})$$

$$\frac{\partial G_{ij\sigma}^{(R)}(t_1, t_2)}{\partial t_1} = \frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial T} + \frac{1}{2} \frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial t} = \frac{1}{2} \frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial t} \quad (\text{B.2})$$

Here we used $\partial T/\partial t_2 = \partial T/\partial t_1 = 1$ and $\partial t/\partial t_1 = -\partial t/\partial t_2 = 1/2$. Moreover, $\frac{\partial G_{ij\sigma}^{(R)}(T_0, t)}{\partial T} = 0$, because we fixed the T_0 instant of time for the Green function. Therefore, with this constraint, we are again in the conditions described in Section II (the derivative with respect to t_1 is opposite than with respect to t_2). We can perform the limiting procedure ($t \rightarrow 0$) and then Fourier transform with respect to the variable t , only, so as to obtain the sum-rule following the same steps as in section II, except that now the Green function depends on the specific time-instant T_0 : $G(T_0, \omega)$. This implies that the sum-rule depends on the time-instant, at variance with the main result of the text when time-translation invariance is imposed. In spite of the remarkable result of this section, the latter point is, after all, obvious: in equilibrium conditions the result is independent of the time-instant by construction (so, no dependence on T should be expected), whereas this is not the case in out-of-equilibrium conditions, where the solution of Eq. (9) explicitly depends on the value of T_0 .

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