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Equation of motion method for composite field operators

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Abstract. The Green's function formalism in Condensed Matter Physics is reviewed within the equation of motion approach. Composite operators and their Green's functions naturally appear as building blocks of generalized perturbative approaches and require fully self-consistent treatments in order to be properly handled. It is shown how to unambiguously set the representation of the Hilbert space by fixing both the unknown parameters, which appear in the linearized equations of motion and in the spectral weights of non-canonical operators, and the zero-frequency components of Green's functions in a way that algebra and symmetries are preserved. To illustrate this procedure some examples are given: the complete solution of the two-site Hubbard model, the evaluation of spin and charge correlators for a narrow-band Bloch system, the complete solution of the three-site Heisenberg model, and a study of the spin dynamics in the Double-Exchange model.

PACS. 71.10.-w Theories and models of many-electron systems – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.10.Fd Lattice fermion models (Hubbard model, etc.)

1 Introduction

The physical system analyzed in this paper is an aggregate of interacting *Wannier*-electrons *living* on a lattice spanned by the vectors $\mathbf{i}$. For the sake of simplicity, we restrict our study to single-band electron models; the generalization to multi-band models is straightforward. The system is enclosed in a finite, but macroscopically large, volume V, containing M sites of the lattice, and is supposed to be in thermodynamic equilibrium at a temperature T. In a second-quantization scheme the dynamics of this system is ruled by a certain Hamiltonian $\hat{H} = \hat{H}[\varphi(i)]$ describing, in complete generality, the free propagation of the electrons and all the interactions among them and with external fields (e.g., electromagnetic fields, pressure and temperature gradients,...). $\varphi(i)$ denotes an Heisenberg electronic field ($i = (\mathbf{i}, t)$) in spinorial notation satisfying canonical anticommutation relations. Any physical property of this system can be connected to the expectation value of a specific operator.

The expectation value $\langle \hat{A} \rangle$ of any operator $\hat{A} = \hat{A}[\varphi(i)]$ can be computed, for the grand-canonical ensemble, by taking the normalized trace of the operator weighted with the quantum-mechanical statistical factor $\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$. $\hat{N} = \sum_{\mathbf{i}\sigma} \varphi^{\dagger}_{\sigma}(i)\varphi_{\sigma}(i)$ is the total number operator, β is the inverse temperature and μ is the chemical potential, which is fixed in order to get the desired average number of particles $N = \langle \hat{N} \rangle$. The chemical potential will be a function of N and T, as well as other parameters present in the Hamiltonian. Although the trace can be taken over any basis (i.e., over any complete set of states in the Hilbert space of the system), the most convenient one, the eigenbasis, is constituted by the simultaneous eigenstates of $\hat{H}$ and $\hat{N}$. If such a basis is known, then all the properties of the system can be exactly calculated: this procedure is known as exact diagonalization (*ED*). It is worth reminding that the Hilbert space of a fermionic system contains only those states compatible with the Pauli principle (i.e., states with occupation numbers per site and spin [1] equal to either 0 or 1).

Generally, *ED* can be effectively applied only to systems that are non-interacting or interacting, but very small. In particular, if the system is non-interacting the eigenbasis coincides with the canonical basis of the Fock space of the system (i.e., the set of states constructed by locating the electrons, one at a time, on the lattice sites in accordance with the Pauli principle). For small systems, it is always possible to exactly diagonalize the Hamiltonian according to the reasonable small number of available states, but when large interacting systems are considered the number of states can be enormous and *ED* is practically not applicable. This consideration gave birth to numerous numerical techniques: Lanczos, quantum Monte Carlo,..., which can be considered as attempts to construct an approximate version of *ED* that could be applied to very large systems. However, these numerical techniques

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have some very severe limitations coming from the unavoidable small number of sites they can treat (the computational time increases exponentially with the number of available states): they cannot give a reliable description of systems with long range interactions; phases presenting long range order of any kind are absolutely unaccessible; the very low resolution in frequency and momentum prevents the applications to systems with relevant low-energy features (e.g., systems that present Kondo-like effects) or with strong spatial-dependence or anisotropy in their physical properties (e.g., systems that have a Fermi surface ill-defined, nodal or with high angular-momentum symmetry). Moreover, the information we get by means of these techniques for a system of a certain size difficultly can be used for a system of bigger size and, even worse, does not give any clear idea of what can happen in the corresponding bulk system.

According to this, we have to find an alternative exact analytical technique that can generate, for large interacting systems, approximate treatments not suffering from the very severe limitations noticed in the numerical methods. In principle, this technique will obviously give the same exact results of *ED*. Coming back to our original problem, the evaluation of the expectation value $\langle \hat{A} \rangle$, it is possible to use the equation of motion

$$\mathrm{i}\frac{\partial}{\partial t}\varphi(i) = \left[\varphi(i), \hat{H}\right] \tag{1.1}$$

in order to derive one or more equations for this quantity or, better, for the corresponding Green's function (see next section). Actually, the equation of motion (1.1) naturally generates higher-order operators (i.e., operators constituted by more and more elementary fields, some of them centered on farther and farther sites from $\mathbf{i}$). The process can be iterated by time-differentiating the newly generated operators and a chain of equations of motion can be constructed. The obtained system of equations of motion closes on a complete set of eigenoperators of the Hamiltonian

$$\mathrm{i}\frac{\partial}{\partial t}\psi\left(\mathbf{i},t\right) = \left[\psi\left(\mathbf{i},t\right), \hat{H}\right] = \sum_{\mathbf{j}} \varepsilon\left(\mathbf{i},\mathbf{j}\right)\psi\left(\mathbf{j},t\right) \tag{1.2}$$

where $\psi(i)$ is a n-component spinorial field and $\varepsilon\left(\mathbf{i},\mathbf{j}\right)$, usually called the energy matrix, is a square matrix of rank n. This approach is known as the equations of motion method (*EM*) and can be applied, obviously giving the same exact results, in all cases where we can also apply *ED*: if the system is non-interacting the original electronic operators $\varphi(i)$ are the eigenoperators of the Hamiltonian; for small systems the number of equations of motion to be solved simultaneously, in order to find the complete set of eigenoperators, is reasonably small and makes the application feasible. When large interacting systems are considered the number of eigenoperators rapidly increases (diverges in the thermodynamic limit) and *EM* cannot be effectively applied just as *ED* could not be. However, the main difference between the two procedures is that *EM* can be still used in some approximation not subject to the severe limitations noticed in the numerical techniques derived from *ED*.

Any approximation derived from *EM* is based on some of the peculiar properties of eigenoperators (some of them are reported below). These properties are obviously not enjoined by eigenstates that have to be considered always as a whole (symmetry considerations can only reduce a brute force diagonalization to a more refined block diagonalization which is in any way unfeasible in the thermodynamic limit). The iterated process of time-differentiation generates more and more *delocalized* eigenoperators in direct space (i.e., eigenoperators containing original fields siting on more and more distant sites), which are less and less relevant as they have eigenenergies rapidly decreasing with the spatial size of the eigenoperator (i.e., with the maximum distance among the sites where the constituting original fields are sited). Although the total number of eigenoperators is equivalent to the number of possible transitions among all the eigenstates and, therefore, goes as this latter number squared (i.e., if the number of eigenstates is n, then the number of eigenoperators is $\frac{n(n+1)}{2}$), to study a specific physical property we need only to analyze the dynamics of the few eigenoperators relevant to it. Furthermore, the eigenoperators can be easily generalized to any size of the system and the dynamics of all sites can be studied at once; this is impossible for the eigenstates. According to this, for very small clusters too, where the application of *ED* requires undoubtedly less effort than that of *EM*, *EM* solution is preferable as it has the fundamental property to be scalable (i.e., it gives a lot of information about both *EM* solution of bigger clusters and the approximate *EM* solution of the corresponding bulk system).

The line of thinking described so far follows the developments of the condensed matter physics in the last decades. Both *ED* and *EM* try to *diagonalize* the Hamiltonian under study, but in two different spaces. The former searches for the eigenbasis within the Hilbert space of the system, the latter seeks an operatorial basis within the field space generated by the application of the Hamiltonian to the original field and to its *bosonic* aggregations (i.e., to fields constructed by an even number of original fields). While the states of a system drastically change with its size (i.e., the corresponding Hilbert spaces do not overlap), the operators just increase in number and complexity (i.e., the new field space include the old one). Moreover, the relevance of an eigenoperator, which is *measured* by the magnitude of the scale of energy it describes, usually survives any change in size of the system. We can also define as minimal cluster the smallest one allowing all the terms of the Hamiltonian to act properly. Only eigenoperators obtained for systems realized on clusters at least equal to the minimal one can be trusted and used to describe properties of the corresponding bulk systems.

In order to construct any approximation scheme in the framework of *EM*, a convenient generalization of the concept of correlation function is provided by that of Green's function [2] (*GF*). The latter has some advantages in the construction and solution of the equations that determine

it. Moreover, the *GF* contain most of, practically all, the relevant information on the properties of the system: expectation values of observables, excitation spectrum, response to external perturbations, and so on. Different types of *GF* can be constructed; we will consider real-time thermodynamic *GF* where the thermal averaging process of the Heisenberg operators is performed over the grand-canonical ensemble.

The traditional approximation schemes, often based on perturbative calculations, use as building blocks the non-interacting *GF*. The mean-field formulation, which corresponds to the linearization of the equation of motion (1.1) (i.e., $\mathrm{i}\frac{\partial}{\partial t}\varphi(\mathbf{i},t) = \sum_{\mathbf{j}} \varepsilon(\mathbf{i},\mathbf{j})\,\varphi(\mathbf{j},t)$, where $\varepsilon(\mathbf{i},\mathbf{j})$ is now a scalar function), also belongs to this category. An intense study has been performed along this line and many techniques have been set up: perturbation expansions on the basis of Feynman diagrams, Dyson equation, Wick's theorem, and so on. It is worth noting that in order to describe phases with different symmetries, these schemes need to become self-consistent.

All these techniques rely on the hypothesis that the interactions among the electrons are weak and can be treated in the framework of some perturbation scheme. However, as many and many theoretical and experimental studies have shown with more and more convincing evidence, all these methods are not adequate to treat strongly correlated electron systems (*SCES*) and different approaches must be considered. In these systems, the fundamental concept of the electron as a particle with some well-defined properties completely breaks down. The presence of the correlations modifies the properties of the electrons and, at the macroscopic level, new particles are observed, with peculiar properties entirely determined by the dynamics and the boundary conditions (i.e., all the elements characterizing the physical situation we wish to study). These new objects appear as the final result of the modifications imposed on the electrons by the interactions and contain, by the very beginning, a relevant part of the effects of correlation.

As simple, but significative, example, let us consider an atomic model with a local interaction U between the electrons (i.e., $\hat{H} = U\varphi_{\uparrow}^{\dagger}\varphi_{\uparrow}\varphi_{\downarrow}^{\dagger}\varphi_{\downarrow}$). This model is exactly solvable in terms of the Hubbard operators

$$\begin{aligned} \xi &= \left[1 - \varphi^{\dagger}\varphi\right]\varphi \\ \eta &= \left[\varphi^{\dagger}\varphi\right]\varphi. \end{aligned} \tag{1.3}$$

Due to the presence of the local interaction U, the original electrons $\varphi(i)$ are no more observables and new stable elementary excitations, described by the field operators $\xi(i)$ and $\eta(i)$, appear.

On the basis of this evidence, one can be induced to move the attention from the original fields to the new fields generated by the interactions. The operators describing these excitations can be written in terms of the original ones and are known as composite operators. Several approaches have been formulated where composite fields are used as operatorial basis for developing approximation schemes [3–14]. All these approaches are very promising: some amount of the interaction is already present in the chosen basis and this permits to overcome the problem of finding an appropriate expansion parameter. However, a price must be paid. In general, the composite fields are neither Fermi nor Bose operators, since they do not satisfy canonical (anti)commutation relations, and their properties, because of the inherent definition, must be self-consistently determined. They can only be recognized as fermionic or bosonic according to the number of constituting original particles.

New techniques of calculus have to be used in order to deal with composite fields. In developing approximation schemes where the building blocks are now the propagators of composite operators, one cannot use the standard version of the consolidated schemes; diagrammatic expansions, Wick's theorem and many other prescriptions are no more valid for composite operators. There have been attempts [15–17] to extend these schemes, but although very good results have been obtained for spin operators [15], the complexity (and often the ambiguity) of the analytical calculations required by the Hubbard operators (the simpler among the fermionic composite operators) does not allow, at least at the present, an effective application of such techniques to real problems. The formulation of the *GF* method must be revisited. As it will be shown below, three serious problems arise when we wish to study the propagators of composite fields:

1. the appearance of some unknown parameters as correlation functions of field operators not belonging to the chosen operatorial basis;
2. the appearance of some zero-frequency constants (*ZFC*) as a consequence of the existence of zero-frequency modes;
3. the necessity of fixing the representation where the *GF* are formulated.

In most of the approaches found in the literature the solution to the previous problems is the following.

1. In order to determine the unknown parameters several methods (arbitrary ansatz, decoupling schemes, use of the equation of motion, ...) have been considered in the context of different approaches (Hubbard I approximation, Roth's method, projection method, spectral density approach, ...). All these methods suffer from the severe limitation of not being fully self-consistent. On the other hand, any approach based on the correct use of composite operators is, by construction, a fully self-consistent approach. As shown in reference [13], in the context of the Hubbard model, all these procedures lead to a series of unpleasant results: several sum rules and the particle-hole symmetry are violated, there is no presence of a Mott transition, all local quantities strongly disagree with the results of the numerical simulation.

2. Any symmetry enjoined by the Hamiltonian induces a degeneracy among the eigenstates of the system. The equivalence of two or more eigenenergies implies the presence of zero-energy modes. In the case of bosonic Green's functions these modes give rise to some unknown quantities that we will call *ZFC*. The *ZFC* are really relevant quantities as they are connected to fundamental physical properties such as the compressibility and the specific

heat: they can be considered as a measure of the fluctuations, quantum and/or thermal ones, present in the thermal averages of the generators of the symmetry group, which are usually bosonic. The *ZFC* are usually fixed by requiring the ergodicity of the dynamics of the relative operators with respect to the Hamiltonian under study. This is clearly a very strong assumption. As it will be shown in the third section of this paper, there are non-trivial examples of exactly-solvable systems where the *ZFC* do not assume their ergodic value: if we would have forced the *ZFC* to assume it, this would have implied a zero compressibility, specific heat,... Furthermore, although the response functions do not explicitly depend on them, there is an implicit dependence due to the inherent self-consistency of the entire scheme. According to this, in general, these quantities must be calculated case by case.

3. The knowledge of the Hamiltonian and of the operatorial algebra is not sufficient to completely specify the *GF*. The *GF* refer to a specific representation (i.e., to a specific choice of the Hilbert space) and this information must be supplied to the equations of motion that alone are not sufficient to completely determine the *GF*. As well known, the same system can exist in different phases according to the external conditions; the existence of infinite inequivalent representations [18] where the equations of motions can be realized, allows us to pick up, among the many possible choices, the right Hilbert space appropriate to the physical situation under study. The construction of the Hilbert space where the *GF* are realized is not an easy task and is usually ignored. The use of composite operators leads to an enlargement of the Hilbert space by the inclusion of some unphysical states. As a consequence of this, it is difficult to satisfy a priori all the sum rules and, in general, the symmetry properties enjoined by the system under study. In addition, since the representation where the operators are realized has to be dynamically determined, the method clearly requires a process of self-consistency.

In the Composite Operator Method [12,13] (*COM*), as illustrated in the next Section, the three problems are not considered separately but they are all connected in one self-consistent scheme. The main idea is that fixing the values of the unknown parameters and of the *ZFC* implies to put some constraints on the representation where the *GF* are realized. As the determination of this representation is not arbitrary, it is clear that there is no freedom in fixing these quantities. They must assume values compatible with the dynamics and with the right representation. Which is the right representation? This is a very hard question to answer. From the algebra it is possible to derive several relations among the operators (e.g., $\varphi_\sigma(i)\varphi_\sigma(i) = 0$): we will call them Algebra Constraint relations (*AC*). This set of relations, valid at microscopic level, must be satisfied also at macroscopic level (i.e., when the expectations values are considered; e.g., $\langle\varphi_\sigma(i)\varphi_\sigma(i)\rangle = 0$). We also note that in general the Hamiltonian has some symmetry properties (e.g., rotational invariance in coordinate and spin space, phase invariance, gauge invariance, ...). These symmetries generate a set of relations among the n-point Green's functions: the Ward-Takahashi relations [19] (*WT*). It is worth noting that many approximations present in the literature do not fulfill these consistency requirements and, consequently, obtain *wrong* results. Now, certainly the right representation must be the one where all relations among the operators satisfy the conservation laws present in the theory when expectation values are taken (i.e., where all the *AC* and *WT* are preserved). Then, we impose these conditions and obtain a set of self-consistent equations that will fix the unknown correlators, the *ZFC* and the right representation at the same time, avoiding the problem of *uncontrolled* and *uncontrollable* decouplings, which affects many different approximation schemes and has been here definitely solved. This is the main ingredient of the *COM*, together with the recipes [20] that we have developed in the last years in order to choose the appropriate operatorial basis of composite operators according to the specific system under analysis. As regards this last issue, we wish to drive the attention on the procedure we propose as it can be considered a systematic attempt to seek and build up (exact as much as it is possible) operatorial basis for interacting systems. This is a new frontier in condensed matter theory (quantum Hall effect, heavy-fermion systems, quantum critical points, competing unconventional ordering phenomena, breakdown of Fermi liquid picture, connections among spin, charge, orbital and lattice degrees of freedom, ...) and our procedure should be regarded as an attempt to revisit the established picture for strongly correlated systems.

The second section is devoted to revisit the *GF* formalism in presence of composite fields and to establish the *COM* as a general procedure to compute *GF* of highly correlated systems. In the third section of the paper we will illustrate the formalism by considering some specific examples: the two-site Hubbard model, the three-site Heisenberg model, a narrow-band Bloch system in presence of an external magnetic field and the double-exchange model. For the two-site Hubbard model we compute the fermionic *GF* independently from the bosonic one by means of the *AC*. The latter also allow us to fix the *ZFC* of the bosonic *GF*, which result in not being ergodic, and to get straightforwardly the right representation. The solution of the tree-site Heisenberg model shows the impossibility to get any spontaneously ordered state at finite temperature in a finite system as a consequence of internal consistency in the proposed formulation. Moreover, it is really relevant the existing relation between the number of *ZFC* appearing in the *GF* and the presence of the magnetic field. In the case of a narrow-band Bloch system in presence of an external magnetic field we will see that the *ZFC* relative to the total number operator, which is an integral of motion, has a non-ergodic value, even if we have an ergodic charge dynamics. The double-exchange model finally gives us the possibility to show one way to apply the proposed formulation to large interacting systems. In this case, we also show how to recognize the manifestation of the Mermin-Wagner theorem [21] within this formulation. For the exactly-solvable models used in the

examples (i.e., the Hubbard and the Heisenberg models), we have checked, although it could not be otherwise, that the proposed formulation reproduces the exact results coming from *ED*. Actually, the *COM* has been developed just for systems large and interacting; the applications to systems that are small or non-interacting have only to be interpreted as mere demonstrations of all features of the method and of its power and correctness. Finally, in the Appendices, we give: a generalized perturbative approach for strongly interacting systems; part of the derivation of the general formulation; the derivation of the zero-temperature formulation; the *GF* expressions, dispersion relations and sum rules where the presence of the *ZFC* is explicitly taken into account.

2 General formalism

This section is devoted to revisit the *GF* formalism in presence of composite fields and to establish the *COM* as a general procedure to compute *GF* of complex interacting systems. Owing to the difficulties in dealing with composite operators, reported in detail in the previous section, the study is performed completely within *EM*. We start by considering a set of composite fields, chosen according to a well-defined recipe [20]. The fields can be of fermionic or bosonic nature, according to the physical properties we wish to study [22]. In the case of fermionic operators it is intended that we use the spinorial representation. The set $\psi(i)$ satisfies a linear system of equations of motion (see Eq. (1.2)). If the fields $\psi(i)$ are eigenoperators of the total Hamiltonian, the equations of motion are exact. Several examples will be given in Section 3. If the fields $\psi(i)$ are not eigenoperators of the Hamiltonian, the equations of motion are approximated and all the formalism is developed with the aim of computing and using the propagators of these fields as a basis to set up a perturbative scheme of calculations. In Appendix A, we give a sketch of a generalized perturbative approach based on a Dyson equation (Eq. (A.5)) designed for formulations using composite fields. Then, the total weight of the self-energy corrections is bounded by the weight of the residual source operator $\delta J(i)$ (see Eq. (A.2)). According to this, it can be made smaller and smaller by increasing the components of the basis $\psi(i)$ (e.g., by including higher-order composite operators appearing in $\delta J(i)$). The result of such procedure will be the inclusion in the energy matrix of part of the self-energy as an expansion in terms of coupling constants multiplied by the weights of the newly included basis operators. In general, the enlargement of the basis leads to a new self-energy with a smaller total weight. However, it is necessary pointing out that this process can be quite cumbersome and the inclusion of fully momentum and frequency dependent self-energy corrections can be necessary to effectively take into account low-energy and virtual processes. According to this, one can choose a reasonable number of components for the basic set and then use another approximation method to evaluate the residual dynamical corrections (e.g., specially adapted versions of the non-crossing approximation or of the FLEX).

By considering two-time thermodynamic *GF* [2,23,24], let us define the causal function

$$G_C^{(\eta)}(i,j) = \theta(t_i - t_j)\,\langle \psi(i)\,\psi^\dagger(j)\rangle - \eta\,\theta(t_j - t_i)\,\langle \psi^\dagger(j)\,\psi(i)\rangle \quad (2.1)$$

the retarded and advanced functions

$$G_{R,A}^{(\eta)}(i,j) = \pm\theta[\pm\,(t_i - t_j)]\,\left\langle \left[\psi(i),\,\psi^\dagger(j)\right]_\eta \right\rangle \quad (2.2)$$

and the correlation function

$$C(i,j) = \langle \psi(i)\,\psi^\dagger(j)\rangle\,. \quad (2.3)$$

Here $\eta = \pm 1$; usually, it is convenient to take $\eta = 1$ ($\eta = -1$) for a *fermionic* (*bosonic*) set $\psi(i)$ (i.e., for a composite field constituted of an odd (even) number of original fields $\varphi(i)$) in order to exploit the canonical anticommutation relations satisfied by $\varphi(i)$; but, in principle, both choices are possible. Accordingly, we define

$$[A,\,B]_\eta = \begin{cases} \{A,\,B\} = A\,B + B\,A & \text{for } \eta = 1 \\ [A,\,B] = A\,B - B\,A & \text{for } \eta = -1 \end{cases} \quad (2.4)$$

$\langle \cdots \rangle$ denotes the quantum-statistical average over the grand canonical ensemble. From the equation (1.2) for the set $\psi(i)$, the Fourier transforms of these functions satisfy the following equations (we consider a translational invariant system)

$$[\omega - \varepsilon(\mathbf{k})]\,G_{C,R,A}^{(\eta)}(\mathbf{k},\omega) = I^{(\eta)}(\mathbf{k}) \quad (2.5a)$$

$$[\omega - \varepsilon(\mathbf{k})]\,C(\mathbf{k},\omega) = 0 \quad (2.5b)$$

where

$$I^{(\eta)}(\mathbf{k}) = \mathcal{F}\left\langle \left[\psi(\mathbf{i},t),\,\psi^\dagger(\mathbf{j},t)\right]_\eta \right\rangle \quad (2.6)$$

is known as the normalization matrix. $\mathcal{F}$ indicates the Fourier transform. The most general solution of equations (2.5) is

$$G_{C,R,A}^{(\eta)}(\mathbf{k},\omega) = \sum_{l=1}^{n} \left\{ \mathcal{P}\left[\frac{\sigma^{(\eta,l)}(\mathbf{k})}{\omega - \omega_l(\mathbf{k})}\right] - \mathrm{i}\,\pi\,\delta[\omega - \omega_l(\mathbf{k})]\; g_{C,R,A}^{(\eta,l)}(\mathbf{k}) \right\} \quad (2.7a)$$

$$C(\mathbf{k},\omega) = \sum_{l=1}^{n} \delta[\omega - \omega_l(\mathbf{k})]\; c^{(l)}(\mathbf{k}) \quad (2.7b)$$

$g_{C,R,A}^{(\eta,l)}(\mathbf{k})$ and $c^{(l)}(\mathbf{k})$ are not fixed by the equations of motion and have to be determined by imposing the appropriate *boundary conditions*. $\omega_l(\mathbf{k})$ are the eigenvalues of the matrix $\varepsilon(\mathbf{k})$. $\sigma^{(\eta,l)}(\mathbf{k})$ are the spectral density functions and can be expressed in terms of the matrices $\varepsilon(\mathbf{k})$ and $I^{(\eta)}(\mathbf{k})$ as

$$\sigma_{\alpha\beta}^{(\eta,l)}(\mathbf{k}) = \Omega_{\alpha l}(\mathbf{k}) \sum_{\delta} \Omega_{l\delta}^{-1}(\mathbf{k})\, I_{\delta\beta}^{(\eta)}(\mathbf{k}) \quad (2.8)$$

where $\Omega(\mathbf{k})$ is the $n \times n$ matrix whose columns are the eigenvectors of the matrix $\varepsilon(\mathbf{k})$. The summations run over the number of eigenvalues of $\varepsilon(\mathbf{k})$ and $\mathcal{P}$ represents the principal value.

By recalling the *boundary conditions* $G_R^{(\eta)}(t<0)=0$ and $G_A^{(\eta)}(t>0)=0$ it is immediate to see that

$$g_R^{(\eta,l)}(\mathbf{k}) = -g_A^{(\eta,l)}(\mathbf{k}) = \sigma^{(\eta,l)}(\mathbf{k}). \tag{2.9}$$

Then, the retarded and advanced *GF* are completely determined in terms of the matrices $\varepsilon(\mathbf{k})$ and $I^{(\eta)}(\mathbf{k})$.

The determination of $g_C^{(\eta,l)}(\mathbf{k})$ and $c^{(l)}(\mathbf{k})$ require some more work. On the basis of the calculations reported in Appendix B, it is straightforward to obtain the following results

$$\sum_{l\in\mathcal{A}(\mathbf{k})} g_C^{(\eta,l)}(\mathbf{k}) = (1-\eta)\Gamma(\mathbf{k}) \tag{2.10a}$$

$$\sum_{l\in\mathcal{A}(\mathbf{k})} \sigma^{(1,l)}(\mathbf{k}) = (1+\eta)\Gamma(\mathbf{k}) \tag{2.10b}$$

$$c^{(l)}(\mathbf{k}) = \frac{2\pi}{1+\eta\, e^{-\beta\,\omega_l(\mathbf{k})}}\sigma^{(\eta,l)}(\mathbf{k}) \quad \forall l\in\mathcal{B}(\mathbf{k}) \tag{2.10c}$$

$$g_C^{(\eta,l)}(\mathbf{k}) = \frac{1-\eta\, e^{-\beta\,\omega_l(\mathbf{k})}}{1+\eta\, e^{-\beta\,\omega_l(\mathbf{k})}}\sigma^{(\eta,l)}(\mathbf{k}) \quad \forall l\in\mathcal{B}(\mathbf{k}) \tag{2.10d}$$

where $\mathcal{A}(\mathbf{k})$ and $\mathcal{B}(\mathbf{k})$ are explicitly defined in equation (B.4) and $\Gamma(\mathbf{k})$, the zero-frequency function, is defined as

$$\Gamma(\mathbf{k}) = \frac{1}{2\pi}\sum_{l\in\mathcal{A}(\mathbf{k})} c^{(l)}(\mathbf{k}). \tag{2.11}$$

We see that equation (2.10b) requires that

$$\sum_{l\in\mathcal{A}(\mathbf{k})} \sigma^{(-1,l)}(\mathbf{k}) = 0. \tag{2.12}$$

This condition comes from the requirement that the correlation function in direct space should not diverge: a solution with $\sum_{l\in\mathcal{A}(\mathbf{k})}\sigma^{(-1,l)}(\mathbf{k}) \neq 0$ implies a divergence of the Fourier coefficients $c^{(l)}(\mathbf{k})$ for any finite temperature. This is admissible only if the divergence is integrable and the corresponding direct space correlation function remains finite. A finite value of $\sum_{l\in\mathcal{A}(\mathbf{k})}\sigma^{(-1,l)}(\mathbf{k})$ is generally related to the presence of long-range order (i.e., symmetry breaking) and the previous statement is nothing but the Mermin-Wagner theorem [21]. A detailed analysis of this point will be illustrated in Section 3 by investigating the Heisenberg and Double Exchange Models.

By putting equations (2.9) and (2.10) into equations (2.7) we get the following general expressions for the *GF*

$$G_{R,A}^{(\eta)}(\mathbf{k},\omega) = \sum_{l\in\aleph}\frac{\sigma^{(\eta,l)}(\mathbf{k})}{\omega-\omega_l(\mathbf{k})\pm \mathrm{i}\,\delta} \tag{2.13a}$$

$$\begin{aligned} G_C^{(\eta)}(\mathbf{k},\omega) = {} & \Gamma(\mathbf{k})\left(\frac{1}{\omega+\mathrm{i}\,\delta}+\frac{\eta}{\omega-\mathrm{i}\,\delta}\right) \\ & + \sum_{l\in\mathcal{B}(\mathbf{k})}\frac{\sigma^{(\eta,l)}(\mathbf{k})}{1+\eta\, e^{-\beta\omega}} \\ & \times\left[\frac{1}{\omega-\omega_l(\mathbf{k})+\mathrm{i}\,\delta}+\frac{\eta\, e^{-\beta\,\omega}}{\omega-\omega_l(\mathbf{k})-\mathrm{i}\,\delta}\right] \end{aligned} \tag{2.13b}$$

$$\begin{aligned} C(\mathbf{k},\omega) = {} & 2\pi\,\delta(\omega)\,\Gamma(\mathbf{k}) \\ & + 2\pi\sum_{l\in\mathcal{B}(\mathbf{k})}\delta[\omega-\omega_l(\mathbf{k})]\,\frac{\sigma^{(\eta,l)}(\mathbf{k})}{1+\eta\, e^{-\beta\,\omega_l(\mathbf{k})}}. \end{aligned} \tag{2.13c}$$

As shown in Appendix C, equations (2.13) hold also in the limit of zero temperature (i.e., in the limit $\beta\to\infty$). From these expressions it is possible to get dispersion relations and sum rules that take explicitly into account the presence of the zero-frequency function (see Appendix D).

We see that the general structure of the *GF* is remarkably different according to the statistics. For *fermionic* composite fields (i.e., when it is natural to choose $\eta=1$) the zero-frequency function $\Gamma(\mathbf{k})$ contributes to the spectral function, it is directly related to the spectral density functions by means of equation (2.10b) and its calculation does not require more information. For *bosonic* composite fields (i.e., when it is natural to choose $\eta=-1$) the zero-frequency function does not contribute to the spectral function, but to the imaginary part of the causal *GF*. The causal and retarded (advanced) *GF* contain different information and the right procedure of calculation is controlled by the statistics. In particular, in the case of bosonic fields (i.e., for $\eta=-1$) one must start from the causal function and then use

$$\begin{aligned} \Re\left[G_{R,A}^{(-1)}(\mathbf{k},\omega)\right] &= \Re\left[G_C^{(-1)}(\mathbf{k},\omega)\right] \\ \Im\left[G_{R,A}^{(-1)}(\mathbf{k},\omega)\right] &= \pm\tanh\frac{\beta\,\omega}{2}\,\Im\left[G_C^{(-1)}(\mathbf{k},\omega)\right] \\ C(\mathbf{k},\omega) &= -\left[1+\tanh\frac{\beta\,\omega}{2}\right]\Im\left[G_C^{(-1)}(\mathbf{k},\omega)\right]. \end{aligned} \tag{2.14}$$

On the contrary, for fermionic fields (i.e., for $\eta=1$) the right procedure for computing the correlation function requires first the calculation of the retarded (advanced) function and then the use of relations identical to those of equations (2.14), but with the subscript R,A and C inverted and the minus sign in the last equation changed to $\mp$.

Moreover, it is worth noting that $\Gamma(\mathbf{k})$ is undetermined within the *bosonic* sector (i.e., for $\eta=-1$) and should be computed in the *fermionic* sector (i.e., for $\eta=1$) by

means of equation (2.10b) or equivalently by means of the following relation

$$\Gamma(\mathbf{k}) = \frac{1}{2} \lim_{\omega \to 0} \omega \, G_C^{(1)}(\mathbf{k}, \omega). \tag{2.15}$$

However, the calculation of $\sigma^{(1,l)}(\mathbf{k})$ requires the calculation of $I^{(1)}(\mathbf{k})$ that, for *bosonic* fields, generates unknown momentum dependent correlation functions whose determination can be very cumbersome as requires, at least in principle, the self-consistent solution of the integral equations connecting them to the corresponding Green's functions. In practice, also for simple, but anyway composite, *bosonic* fields the $\Gamma(\mathbf{k})$ remains undetermined and other methods rather than equation (2.10b) should be used. Similar methods, like the use of the relaxation function [25], would lead to the same problem.

The zero-frequency function $\Gamma(\mathbf{k})$ is known in the literature [25–31] as an indicator of the ergodic nature of the dynamics of the operator $\psi(i)$ with respect to the Hamiltonian $\hat{H}$. We recall that a quantity A has an ergodic dynamics if and only if

$$\lim_{t \to \infty} \langle A(t) \, A \rangle = \langle A \rangle^2 \tag{2.16}$$

that is, if and only if its auto-correlation attenuates in the time. We have not to forget that the condition (2.16) is the same as the standard ergodic requirement (i.e., equivalence of averages taken in time and over the phase space) only for statistical averages computed in the microcanonical ensemble [25]; in other ensembles it holds only in the thermodynamic limit. By recalling the general expression (2.13c) for the correlation function, the condition of ergodic dynamics for $\psi(i)$ is

$$\frac{1}{M} \sum_{\mathbf{k}} e^{\mathrm{i}\,\mathbf{k}(\mathbf{i}-\mathbf{j})} \, \Gamma(\mathbf{k}) = \langle \psi(\mathbf{i}) \rangle \, \langle \psi^\dagger(\mathbf{j}) \rangle \, . \tag{2.17}$$

It is worth noting that $\Gamma(\mathbf{k})$ generally does not assume its ergodic value (i.e., that required by Eq. (2.17)) and has to be computed case by case according to the dynamics and the boundary conditions. For instance, for any finite system the statistical ensembles are not equivalent and the criterion (2.16) holds only in the microcanonical one. Moreover, the condition (2.16) is not satisfied by any integral of motion or, more generally, by any operator that has a diagonal part with respect to the Hamiltonian under study [27] (i.e., by any operator that has diagonal entries whenever written in the basis of the eigenstates of the Hamiltonian under study). This latter consideration clarifies why the ergodic nature of the dynamics of an operator mainly depends on the Hamiltonian it is subject to. It is really remarkable that the zero-frequency constants (*ZFC*), which are the values of the zero-frequency function $\Gamma(\mathbf{k})$ over the momenta for which $\mathcal{A}(\mathbf{k}) \neq \emptyset$, are directly related to relevant measurable quantities such as the compressibility, the specific heat, the magnetic susceptibility,... For instance, we recall the formula that relates the compressibility to the total particle number fluctuations

$$\kappa = \beta \frac{M}{N^2} \left[\langle \hat{N}^2 \rangle - N^2 \right]. \tag{2.18}$$

According to this, in the case of infinite systems too the correct determination of the *ZFC* cannot be considered as an irrelevant issue (e.g., Eq. (2.18) holds in the thermodynamic limit too). In conclusion, equation (2.17) generally cannot be used to compute the *ZFC*. In the next section, we provide some examples of violation of the condition (2.16). It is necessary pointing out, in order to avoid any possible confusion to the reader, that we are using (here and in the examples presented in the next section) *full* operators and not *fluctuation* ones (i.e., we use operators not diminished of their average value, in contrast with what it is usually done for the bosonic excitations like spin, charge and pair). According to this, the *ZFC* can be different from zero (i.e., be equal to the squared average of the operator), and still indicate an ergodic dynamics for the operator.

Summarizing, by means of *EM* and by using the boundary conditions relative to the original definitions of the various *GF* we have been able to derive explicit expressions for these latter (see Eqs. (2.13)). However, these expressions can only determine the functional dependence of the *GF*: their knowledge is not fully achieved yet. According to the (anti)commutation relations, the normalization matrix $I^{(\eta)}(\mathbf{k})$ usually contains some unknown functions that have to be self-consistently calculated together with the *ZFC* (and the energy matrix $\varepsilon(\mathbf{k})$ if we use some approximation scheme). These functions are static correlation functions (correlators since now on) of operators not belonging to the chosen basis. In principle, one could introduce a new set of composite fields and repeat all scheme of calculations in order to calculate the unknown correlators. However, the new set will possibly generate other unknown correlators and the entire process of self-consistency might become very cumbersome and, in most of the cases, not convergent. An alternative scheme of calculation can be proposed. Fixing the values of the unknown parameters and of the *ZFC* implies to put some constraints on the representation where the *GF* are realized. As the determination of this representation is not arbitrary, it is clear that there is no freedom in fixing these quantities. They must assume values compatible with the dynamics and with the right representation. Now, certainly the right representation must be the one where all relations among the operators are systematically conserved when the expectation values are taken (i.e., where all the *AC* and *WT* are satisfied). It is then clear that a shortcut in the procedure of self-consistency can be introduced. We can fix the representation by requiring that

$$\left\langle \psi(i) \, \psi^\dagger(i) \right\rangle = \frac{1}{M} \sum_{\mathbf{k}} \frac{1}{2\pi} \int d\omega \, C(\mathbf{k}, \omega) \tag{2.19}$$

where the l.h.s. is fixed by the *AC*, the *WT* and the boundary conditions compatible with the phase under investigation and in the r.h.s. the correlation function $C(\mathbf{k}, \omega)$ is computed by means of equation (2.13c). Equations (2.19) generate a set of self-consistent equations which determine the unknown parameters (i.e., *ZFC* and unknown correlators) and, consequently, the proper representation [12,13,32]. It is worth noticing that the number

of constraints generated by equation (2.19) can be different from the number of unknowns parameters. Generally, the coincidence of these two numbers signals that the chosen basic set gives a reasonable description of the dynamics contained in the truncated *EM*. Condition (2.19) can be considered as a generalization, to the case of composite fields, of the equation that, in the non-interacting case, fixes the way of counting the particles per site, according to the algebra, by determining the chemical potential. According to this, the unknown correlators, coming from the non-canonical (anti)commutation relations, have not be seen like obstacles as many analytical techniques do, but like a possibility to fix the representation and satisfy all the symmetry relations. Any approximation not using them to do so will surely fail in reproducing the physics of the system under study. It is worth noting, and the examples of the next section will show how, that by means of equation (2.19) is often possible to close one sector (i.e., fermionic, spin, charge, pair, ...) at a time without resorting to the opening of all or many of them simultaneously. Obviously, this occurrence enormously facilitates the calculations. Finally, it is worth noting that the entire process of self-consistency (i.e., the use of Eq. (2.19)) will affect all the *GF* at the same time and, therefore, all the physical properties of the system. For instance, the linear response of the system to an external perturbation (susceptibility, conductivity, ...) is described by two-time retarded *GF* [25]. Although these type of *GF* do not explicitly depend on the *ZFC*, there is an implicit dependence through the internal self-consistent parameters, that is the unknown correlators.

In this section, we have presented the general framework of the *COM*, which results to be a general method to deal with composite fields and, consequently, with complex correlated systems. In the next section, we will illustrate this calculation scheme by considering some specific examples.

3 Examples

3.1 The two-site Hubbard model

The two-site Hubbard model is described by the following Hamiltonian

$$H = \sum_{ij} (t_{ij} - \delta_{ij}\,\mu)\, c^\dagger(i)\, c(j) + U \sum_i n_\uparrow(i)\, n_\downarrow(i) \quad (3.1)$$

where the summation range only over two sites at distance a from each other and the rest of notation is standard [33]. The hopping matrix t_{ij} is defined by

$$t_{ij} = -2t\,\alpha_{ij} \qquad \alpha_{ij} = \frac{1}{2}\sum_k e^{\mathrm{i}\,k(i-j)}\,\alpha(k) \quad (3.2)$$

where $\alpha(k) = \cos(ka)$ and $k = 0,\ \pi/a$.

We now proceed to study the system by means of the equation of motion approach and the *GF* formalism [33] described in Section 2. A complete set of fermionic eigenoperators of $\hat{H}$ is the following one

$$\psi(i) = \begin{pmatrix} \xi(i) \\ \eta(i) \\ \xi_s(i) \\ \eta_s(i) \end{pmatrix} \quad (3.3)$$

where

$$\xi(i) = [1 - n(i)]\, c(i) \quad (3.4a)$$

$$\eta(i) = n(i)\, c(i) \quad (3.4b)$$

$$\xi_s(i) = \frac{1}{2}\sigma^\mu\, n_\mu(i)\, \xi^\alpha(i) + \xi(i)\, \eta^{\dagger\alpha}(i)\, \eta(i) \quad (3.4c)$$

$$\eta_s(i) = \frac{1}{2}\sigma^\mu\, n_\mu(i)\, \eta^\alpha(i) + \xi(i)\, \xi^{\dagger\alpha}(i)\, \eta(i). \quad (3.4d)$$

We define $\psi^\alpha(i) = \sum_j \alpha_{ij}\,\psi(j)$ and use the spinorial notation for the field operators. $n_\mu(i) = c^\dagger(i)\,\sigma_\mu\,c(i)$ is the charge ($\mu = 0$) and spin ($\mu = 1, 2, 3$) operator; greek (e.g., μ, ν) and latin (e.g., a, b, k) indices take integer values from 0 to 3 and from 1 to 3, respectively; sum over repeated indices, if not explicitly otherwise stated, is understood; $\sigma_\mu = (1, \vec{\sigma})$ and $\sigma^\mu = (-1, \vec{\sigma})$; $\vec{\sigma}$ are the Pauli matrices. In momentum space the field $\psi(i)$ satisfies the equation of motion

$$\mathrm{i}\frac{\partial}{\partial t}\psi(k,t) = \varepsilon(k)\,\psi(k,t). \quad (3.5)$$

where the energy matrix $\varepsilon(k)$ has the expression

$$\varepsilon(k) = \begin{pmatrix} -\mu - 2t\,\alpha(k) & -2t\,\alpha(k) & -2t & -2t \\ 0 & U-\mu & 2t & 2t \\ 0 & 4t & -\mu + 2t\,\alpha(k) & 4t\,\alpha(k) \\ 0 & 2t & 2t\,\alpha(k) & U-\mu \end{pmatrix}. \quad (3.6)$$

Straightforward calculations, according to the scheme traced in Section 2, show that two correlators

$$\Delta = \left\langle \xi^\alpha(i)\,\xi^\dagger(i)\right\rangle - \left\langle \eta^\alpha(i)\,\eta^\dagger(i)\right\rangle \quad (3.7)$$

$$p = \frac{1}{4}\left\langle n_\mu^\alpha(i)\, n_\mu(i)\right\rangle - \left\langle c_\uparrow(i)\, c_\downarrow(i)\left[c_\downarrow^\dagger(i)\, c_\uparrow^\dagger(i)\right]^\alpha\right\rangle \quad (3.8)$$

appear in the normalization matrix $I(\mathbf{k}) = \mathcal{F}\left\langle\left\{\psi(\mathbf{i},t),\ \psi^\dagger(\mathbf{j},t)\right\}\right\rangle$. Then, the *GF* depend on three parameters: μ, Δ and p. The correlator Δ can be expressed in terms of the fermionic correlation function $C(i,j) = \left\langle\psi(i)\,\psi^\dagger(j)\right\rangle$; the chemical potential μ can be related to the particle density by means of the relation $n = 2\,[1 - C_{11}(i,i) - C_{22}(i,i)]$. The parameter p cannot be calculated in the fermionic sector; it is expressed in terms of correlation functions of the bosonic fields $n_\mu(i)$ and $c_\uparrow(i)\,c_\downarrow(i)$. According to this, the determination of the fermionic *GF* requires the parallel study of bosonic *GF*.

After quite cumbersome calculations, it is possible to see [33] that a complete set of bosonic eigenoperators of $\hat{H}$ in the spin-charge channel is given by

$$B^{(\mu)}(i) = \begin{pmatrix} B_1^{(\mu)}(i) \\ \vdots \\ B_6^{(\mu)}(i) \end{pmatrix} \quad (3.9)$$

where

$$B_1^{(\mu)}(i) = c^\dagger(i)\,\sigma_\mu\,c(i) \tag{3.10}$$
$$B_2^{(\mu)}(i) = c^\dagger(i)\,\sigma_\mu\,c^\alpha(i) - c^{\dagger\alpha}(i)\,\sigma_\mu\,c(i) \tag{3.11}$$
$$B_3^{(\mu)}(i) = d_\mu(i) - d_\mu^\alpha(i) + d_\mu^\dagger(i) - d_\mu^{\dagger\alpha}(i) \tag{3.12}$$
$$B_4^{(\mu)}(i) = d_\mu(i) - d_\mu^\alpha(i) - d_\mu^\dagger(i) + d_\mu^{\dagger\alpha}(i) \tag{3.13}$$
$$B_5^{(\mu)}(i) = f_\mu(i) - f_\mu^\alpha(i) - f_\mu^\dagger(i) + f_\mu^{\dagger\alpha}(i) \tag{3.14}$$
$$B_6^{(\mu)}(i) = f_\mu(i) - f_\mu^\alpha(i) + f_\mu^\dagger(i) - f_\mu^{\dagger\alpha}(i) \tag{3.15}$$

with the definitions:

$$d_\mu(i) = \xi^\dagger(i)\,\sigma_\mu\,\eta^\alpha(i) \tag{3.16}$$
$$f_0(i) = -\eta^\dagger(i)\,\eta(i) - d^\dagger(i)\,d^\alpha(i) + \eta^\dagger(i)\,\eta(i)\,\xi^{\dagger\alpha}(i)\,\xi^\alpha(i) \tag{3.17}$$
$$f_a(i) = \xi^\dagger(i)\,\xi(i)\,n_a^\alpha(i) - \frac{1}{2}\mathrm{i}\,\epsilon_{abc}\,n_b(i)\,n_c^\alpha(i). \tag{3.18}$$

The field $B^{(\mu)}(i)$ satisfies the equation of motion

$$\mathrm{i}\frac{\partial}{\partial t}B^{(\mu)}(k,t) = \kappa(k)\,B^{(\mu)}(k,t) \tag{3.19}$$

where the energy matrix $\kappa(k)$ has the expression

$$\kappa(k) = \begin{pmatrix} 0 & -2t & 0 & 0 & 0 & 0 \\ -4t\,[1-\alpha(k)] & 0 & U & 0 & 0 & 0 \\ 0 & 0 & 0 & U & 2t & 0 \\ 0 & 0 & U & 0 & 0 & 2t \\ 0 & 0 & 8t & 0 & 0 & 0 \\ 0 & 0 & 0 & 8t & 0 & 0 \end{pmatrix}. \tag{3.20}$$

The energy spectra are given by

$$\omega_1(k) = -2t\sqrt{2\,[1-\alpha(k)]} \tag{3.21}$$
$$\omega_2(k) = 2t\sqrt{2\,[1-\alpha(k)]} \tag{3.22}$$
$$\omega_3(k) = -U - 4J_U \tag{3.23}$$
$$\omega_4(k) = -4J_U \tag{3.24}$$
$$\omega_5(k) = 4J_U \tag{3.25}$$
$$\omega_6(k) = U + 4J_U \tag{3.26}$$

where

$$J_U = \frac{1}{8}\left[\sqrt{U^2+64t^2} - U\right]. \tag{3.27}$$

Straightforward calculations according to the scheme given in Section 2 show that the correlation function has the expression

$$C^{(\mu)}(i,j) = \left\langle B^{(\mu)}(i)\,B^{(\mu)\dagger}(j)\right\rangle = \frac{1}{4}\sum_k\sum_{n=1}^{6} e^{\mathrm{i}\,k(i-j)-\mathrm{i}\,\omega_n(k)(t_i-t_j)} \times\left[1+\tanh\frac{\beta\,\omega_n(k)}{2}\right] f^{(n,\mu)}(k) \tag{3.28}$$

where

$$f^{(n,\mu)}(0) = 0 \quad for\ \ n = 3,4,5,6 \tag{3.29a}$$
$$f^{(n,\mu)}(\pi) = \coth\frac{\beta\,\omega_n(\pi)}{2}\sigma^{(n,\mu)}(\pi)\ \ \forall n. \tag{3.29b}$$

Owing to the fact that zero-energy modes appear for $n = 1$, 2 and $k = 0$ (*cf.* Eq. (3.21)), *ZFC* appear in the correlation functions

$$\Gamma^{(\mu)}(0) = \frac{1}{2}\sum_{n=1}^{2} f^{(n,\mu)}(0). \tag{3.30}$$

In principle $\Gamma^{(\mu)}(0)$ could be calculated by means of equation (2.10b); however this would require the calculation of the anticommutators $\left\langle\left\{B^{(\mu)}(i,t),\,B^{(\mu)\dagger}(j,t)\right\}\right\rangle$ which generate correlation functions of higher order giving raise to a chain of *GF* whose closure is not evident. Similar methods, like the use of the relaxation function [25], would lead to the same problem. One might think, as is often done in the literature, to fix this constant by its ergodic value. However, this is not correct as we are in a finite system in the grandcanonical ensemble and the ergodicity condition (2.17) does not hold. For the moment, we can state that this constant remains undetermined.

The spectral density functions $\sigma^{(n,\mu)}(k)$, calculated by means of equation (2.8) depends on a set of parameters which come from the calculation of the normalization matrix $I^{(\mu)}(k) = \mathcal{F}\left\langle\left[B^{(\mu)}(i,t),\,B^{(\mu)\dagger}(j,t)\right]\right\rangle$. In particular, for the (1,1)-component the following parameters appear:

$$C_{12}^\alpha = \left\langle\eta^\alpha(i)\,\xi^\dagger(i)\right\rangle \tag{3.31a}$$
$$C^\alpha = \left\langle c^\alpha(i)\,c^\dagger(i)\right\rangle \tag{3.31b}$$
$$d = \left\langle c_\uparrow(i)\,c_\downarrow(i)\left[c_\downarrow^\dagger(i)\,c_\uparrow^\dagger(i)\right]^\alpha\right\rangle \tag{3.31c}$$
$$\chi_s^\alpha = \left\langle\vec{n}(i)\cdot\vec{n}^\alpha(i)\right\rangle. \tag{3.31d}$$

The parameters C^α and C_{12}^α are related to the fermionic correlation function $C(i,j) = \left\langle\psi(i)\,\psi^\dagger(j)\right\rangle$. The parameter χ_s^α can be expressed in terms of the bosonic correlation function $C^{(\mu)}(i,j) = \left\langle B^{(\mu)}(i)\,B^{(\mu)\dagger}(j)\right\rangle$. In order to use the standard procedure of self-consistency, we need to calculate the parameter d. For this purpose we should open both the pair channel and a double occupancy-charge channel (i.e., we will need the static correlation function $\langle n_\uparrow(i)\,n_\downarrow(i)\,n^\alpha(i)\rangle$). The corresponding calculations are reported in reference [33] where is shown that these two channels do not carry any new unknown *ZFC*. The self-consistence scheme closes; by considering the four channels (i.e., fermionic, spin-charge, pair and double occupancy-charge) we can set up a system of coupled self-consistent equations for all the parameters. However, the *ZFC* $\Gamma^{(\mu)}(0)$ has not been determined yet: we have not definitely fixed the representation of the *GF*.

In conclusion, the standard procedure of self-consistency is very involved and is not able to give a final answer because of the problem of fixing the *ZFC*. This

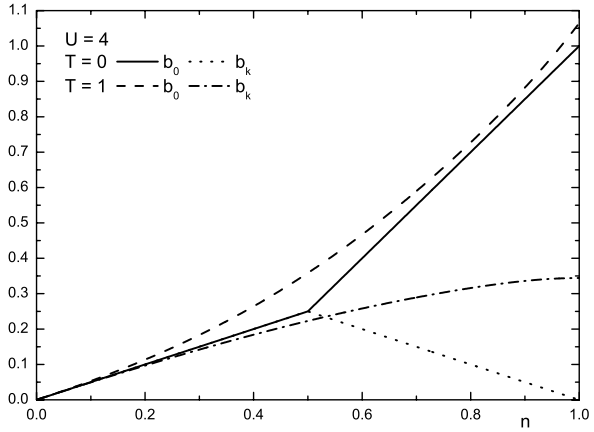

Fig. 1. b_0 and b_k are plotted as functions of n for $U = 4$ and $T = 0$ and 1. U and T are expressed in units of t.

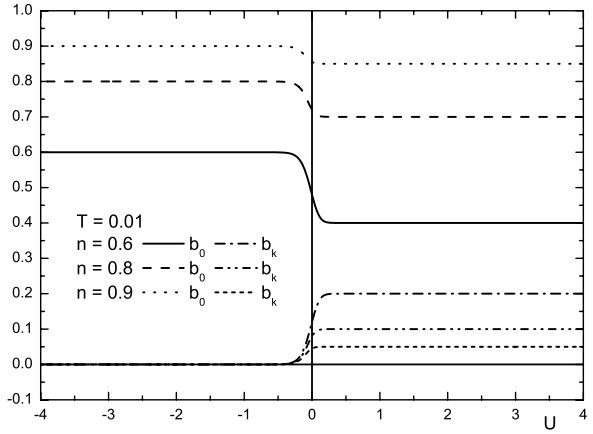

Fig. 2. b_0 and b_k are plotted as functions of U for $T = 0.01$ and $n = 0.6$, 0.8, and 0.9. U and T are expressed in units of t.

problem is known in the literature as the zero-frequency ambiguity of the *GF* formalism [24,26,28–30].

We will now approach the problem by taking a different point of view. The proper representation of the *GF* must satisfy the condition that all the microscopic laws, expressed as relations among operators must hold also at macroscopic level as relations among matrix elements. For instance, let us consider the fermionic channel. We have seen that there exists the parameter p, not explicitly related to the fermionic propagator, that can be determined by opening other channels. However, we know that at the end of the calculations, if the representation is the right one, the parameter p must take a value such that the *symmetries* are conserved. By imposing the AC (2.19) and by recalling the expression for Δ we get three equations

$$n = 2(1 - C_{11} - C_{22}) \tag{3.32a}$$

$$\Delta = C^{\alpha}_{11} - C^{\alpha}_{22} \tag{3.32b}$$

$$C_{12} = 0. \tag{3.32c}$$

This set of coupled self-consistent equations will allow us to completely determine the fermionic *GF*. Calculations show [33] that this way of fixing the representation is the right one: all the *symmetry* relations are satisfied and all the results exactly agree with those obtained by means of *ED*. We do not have to open the bosonic channels; the fermionic one is self-contained.

Next, let us consider the spin-charge *GF*. In the spin-charge sector we have the parameters C^{α}, C^{α}_{12}, χ^{α}_s, d and the two *ZFC*

$$b_0 = \frac{1}{4}\sum_{i=1}^{2} f^{(i,0)}_{11}(0) \tag{3.33}$$

$$b_k = \frac{1}{4}\sum_{i=1}^{2} f^{(i,k)}_{11}(0) \qquad k = 1, 2, 3. \tag{3.34}$$

Since we are in absence of an external applied magnetic field, b_k takes the same values for any value of k.

The parameter C^{α} and C^{α}_{12} are known, since the fermionic correlation functions have been computed. The parameters χ^{α}_s and d can be computed by means of the equations

$$d = \frac{1}{4}\left\langle n^{\alpha}_{\mu}(i)\, n_{\mu}(i)\right\rangle - p \tag{3.35}$$

$$\chi^{\alpha}_s = \langle \vec{n}(i) \cdot \vec{n}^{\alpha}(i)\rangle\,. \tag{3.36}$$

The *ZFC* are fixed by the AC

$$C^{(\mu)}_{11}(i,i) = \langle n_{\mu}(i)\, n_{\mu}(i)\rangle\,. \tag{3.37}$$

By recalling (3.28) and (3.29) we have

$$b_{\mu} = \langle n_{\mu}(i)\, n_{\mu}(i)\rangle - \frac{1}{4}\sum_{i=1}^{6}\left[1 + \coth\frac{\beta\,\omega_i(\pi)}{2}\right]\sigma^{(i,\mu)}_{11}(\pi) \tag{3.38}$$

with

$$\langle n_{\mu}(i)\, n_{\mu}(i)\rangle = \begin{cases} n + 2D \;\; for\;\; \mu = 0 \\ n - 2D \;\; for\;\; \mu = 1, 2, 3. \end{cases} \tag{3.39}$$

$D = \langle n_{\uparrow}(i)\, n_{\downarrow}(i)\rangle$ is the double occupancy and can be calculated by means of the fermionic correlation functions $D = n - 1 + C_{11}$. equations (3.35) and (3.38) constitute a set of coupled self-consistent equations which will determine completely the Green's function in the spin-charge channel. Calculations show that this way of fixing the representation is the right one: all the symmetry relations are satisfied and all the results exactly agree with those obtained by means of *ED*.

The *ZFC* b_0 and b_k are plotted as functions of n and U in Figures 1 and 2, respectively, for various temperatures. It is worth noting that they assume their *ergodic* values (i.e. n^2 and 0, respectively) only in some regions of the parameter space: (at zero temperature) at $n = 1$ (both b_0 and b_k) and at $n = 0.5$ (b_0 only). In these regions, the grand-canonical ensemble is equivalent to the microcanonical one and the underlying ergodicity of the charge and spin dynamics emerges.

It is worth noting that the *ZFC* b_0 is directly related to the compressibility by means of the following relation [33]

$$\kappa = \frac{2}{k_{\mathrm{B}}T}\frac{1}{n^2}\left[b_0 - n^2\right] \tag{3.40}$$

According to this, if we erroneously set the value of b_0 to the ergodic one (i.e., n^2) we would get a constant zero compressibility.

3.2 The three-site Heisenberg model

The three-site Heisenberg model, in presence of an external magnetic field h, is described by the following Hamiltonian

$$\hat{H} = J\sum_{\mathbf{i}=1}^{3} \vec{S}(i)\cdot\vec{S}^{\alpha}(i) - h\sum_{\mathbf{i}=1}^{3} S_z(i) \tag{3.41}$$

where $\vec{S}(i)$ is the local spin at the site $\mathbf{i}$, with quantum number $S=\frac{1}{2}$. The relative positions of the three sites are those of the end-points and the middle-point of a segment, in this case we are using periodic boundary conditions, or those of the vertices of an equilateral triangle; in both cases, the distances of two of them in the given order (i.e., $1\to 2$, $2\to 3$, $3\to 1$) is taken to be unitary. The notation $\vec{S}^{\alpha}(i)$ indicates

$$\vec{S}^{\alpha}(\mathbf{i},t) = \sum_{\mathbf{j}} \alpha_{\mathbf{ij}}\vec{S}(\mathbf{j},t). \tag{3.42}$$

The projection operator $\alpha_{\mathbf{ij}}$ is defined by

$$\alpha_{\mathbf{ij}} = \frac{1}{3}\sum_{k} \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{i}-\mathbf{j})}\alpha(\mathbf{k}) \tag{3.43}$$

$$\alpha(\mathbf{k}) = \cos(\mathbf{k}) \tag{3.44}$$

where $\mathbf{k} = -\frac{2\pi}{3a}$, 0, $\frac{2\pi}{3a}$.

A complete set of eigenoperators of $\hat{H}$ is

$$\psi^{(m)}(i) = \begin{pmatrix} \psi_1^{(m)}(i) \\ \psi_2^{(m)}(i) \\ \psi_3^{(m)}(i) \end{pmatrix} \tag{3.45}$$

where

$$\psi_1^{(m)}(i) = \begin{cases} S^{+}(i) = S_x + \mathrm{i}S_y & \text{for } m=1 \\ S_z(i) & \text{for } m=2 \end{cases} \tag{3.46}$$

$$\psi_2^{(m)}(i) = \begin{cases} l^{+}(i) = l_x + \mathrm{i}l_y & \text{for } m=1 \\ l_z(i) & \text{for } m=2 \end{cases} \tag{3.47}$$

$$\psi_3^{(m)}(i) = \begin{cases} u^{+}(i) = u_x + \mathrm{i}u_y & \text{for } m=1 \\ u_z(i) & \text{for } m=2. \end{cases} \tag{3.48}$$

Hereafter, we will use the two sets of indices $\{x,y,z\}$ and $\{1,2,3\}$ interchangeably.

The composite fields $l_k(i)$ and $u_k(i)$ are defined as

$$l_k(i) = \mathrm{i}\epsilon_{kpq}S_p^{\alpha}(i)S_q(i) \tag{3.49}$$

$$u_k(i) = \mathrm{i}\epsilon_{kpq}[l_p^{\alpha}(i)S_q(i) + S_p^{\alpha}(i)l_q(i)]. \tag{3.50}$$

The field $\psi^{(m)}(i)$ satisfies the equation of motion

$$\mathrm{i}\frac{\partial}{\partial t}\psi^{(m)}(i) = \varepsilon^{(m)}\psi^{(m)}(i) \tag{3.51}$$

where the energy matrix $\varepsilon^{(m)}$ has the expression

$$\varepsilon^{(m)} = \begin{pmatrix} a_m h & 2J & 0 \\ 0 & a_m h & 2J \\ 0 & \frac{9}{8}J & a_m h \end{pmatrix} \tag{3.52}$$

with $a_m = 1-\delta_{2m}$. The energy spectra are given by

$$\omega_1^{(m)} = a_m h \tag{3.53}$$

$$\omega_2^{(m)} = \frac{1}{2}(2a_m h - 3J) \tag{3.54}$$

$$\omega_3^{(m)} = \frac{1}{2}(2a_m h + 3J). \tag{3.55}$$

By means of the equation of motion (3.51), the correlation function

$$C^{(m)}(i,j) = \left\langle \psi^{(m)}(i)\psi^{\dagger(m)}(j)\right\rangle = \frac{1}{3}\sum_{k}\frac{1}{2\pi}\int d\omega\, \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{i}-\mathbf{j})-\mathrm{i}\omega(t_i-t_j)}C^{(m)}(\mathbf{k},\omega) \tag{3.56}$$

has the expression

$$C^{(m)}(\mathbf{k},\omega) = \sum_{n=1}^{3}\delta[\omega-\omega_n^{(m)}(\mathbf{k})]c^{(n,m)}(\mathbf{k}) \tag{3.57}$$

where the matrices $c^{(n,m)}(\mathbf{k})$ have to be calculated.

Straightforward calculations according to the scheme given in Section 2 show that the correlation function is given by

$$C^{(1)}(i,j) = \frac{1}{6}\sum_{n=1}^{3}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{i}-\mathbf{j})-\mathrm{i}\omega_n^{(1)}(k)(t_i-t_j)} \times [1+\coth\left(\frac{\beta\omega_n^{(1)}}{2}\right)]\sigma^{(n,1)}(\mathbf{k}) \tag{3.58}$$

$$C^{(2)}(i,j) = b^{(2)}(\mathbf{i},\mathbf{j}) + \frac{1}{6}\sum_{n=2}^{3}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{i}-\mathbf{j})-\mathrm{i}\omega_n^{(2)}(k)(t_i-t_j)} \times [1+\coth\left(\frac{\beta\omega_n^{(2)}}{2}\right)]\sigma^{(n,2)}(\mathbf{k}) \tag{3.59}$$

where the zero-frequency function

$$b^{(2)}(\mathbf{i},\mathbf{j}) = \frac{1}{2\pi}\frac{1}{3}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{i}-\mathbf{j})}c^{(1,2)}(\mathbf{k}) \tag{3.60}$$

appears owing to the presence of the zero-energy mode $\omega_1^{(2)}=0$.

The spectral density functions $\sigma^{(n,m)}(\mathbf{k})$, calculated by means of equation (2.8), have the following expressions

$$\sigma^{(1,m)}(\mathbf{k}) = \lambda^{(1,m)}(\mathbf{k})A^{(1)} \tag{3.61}$$
$$\sigma^{(2,m)}(\mathbf{k}) = \lambda^{(2,m)}(\mathbf{k})A^{(2)} \tag{3.62}$$
$$\sigma^{(3,m)}(\mathbf{k}) = \lambda^{(3,m)}(\mathbf{k})A^{(3)} \tag{3.63}$$
$$\lambda^{(1,m)}(\mathbf{k}) = I_{11}^{(m)}(\mathbf{k}) - \frac{16}{9}I_{22}^{(m)}(\mathbf{k}) \tag{3.64}$$
$$\lambda^{(2,m)}(\mathbf{k}) = 3I_{12}^{(m)}(\mathbf{k}) - 4I_{22}^{(m)}(\mathbf{k}) \tag{3.65}$$
$$\lambda^{(3,m)}(\mathbf{k}) = 3I_{12}^{(m)}(\mathbf{k}) + 4I_{22}^{(m)}(\mathbf{k}) \tag{3.66}$$

with

$$A^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.67}$$

$$A^{(2)} = \begin{pmatrix} -\frac{2}{9} & \frac{1}{6} & -\frac{1}{8} \\ \frac{1}{6} & -\frac{1}{8} & \frac{3}{32} \\ -\frac{1}{8} & \frac{3}{32} & -\frac{9}{128} \end{pmatrix} \tag{3.68}$$

$$A^{(3)} = \begin{pmatrix} \frac{2}{9} & \frac{1}{6} & \frac{1}{8} \\ \frac{1}{6} & \frac{1}{8} & \frac{3}{32} \\ \frac{1}{8} & \frac{3}{32} & \frac{9}{128} \end{pmatrix}. \tag{3.69}$$

The normalization matrix $I^{(m)}(\mathbf{k}) = \mathcal{F}\left\langle [\psi^{(m)}(\mathbf{i},t), \psi^{\dagger(m)}(\mathbf{j},t)] \right\rangle$, that has the form

$$I^{(1)}(\mathbf{k}) = \begin{pmatrix} I_{11}^{(1)}(\mathbf{k}) & I_{12}^{(1)}(\mathbf{k}) & I_{22}^{(1)}(\mathbf{k}) \\ I_{12}^{(1)}(\mathbf{k}) & I_{22}^{(1)}(\mathbf{k}) & \frac{9}{16}I_{12}^{(1)}(\mathbf{k}) \\ I_{22}^{(1)}(\mathbf{k}) & \frac{9}{16}I_{12}^{(1)}(\mathbf{k}) & \frac{9}{16}I_{22}^{(1)}(\mathbf{k}) \end{pmatrix} \tag{3.70}$$

$$I^{(2)}(k) = \begin{pmatrix} 0 & I_{12}^{(2)}(\mathbf{k}) & 0 \\ I_{12}^{(2)}(\mathbf{k}) & 0 & \frac{9}{16}I_{12}^{(2)}(\mathbf{k}) \\ 0 & \frac{9}{16}I_{12}^{(2)}(\mathbf{k}) & 0 \end{pmatrix} \tag{3.71}$$

with

$$I_{11}^{(1)}(\mathbf{k}) = 2M \tag{3.72}$$
$$I_{12}^{(1)}(\mathbf{k}) = -\left[1-\alpha(\mathbf{k})\right]\left(C_{11}^{(1)\alpha} + 2C_{11}^{(2)\alpha}\right) \tag{3.73}$$
$$I_{12}^{(2)}(\mathbf{k}) = -\left[1-\alpha(\mathbf{k})\right]C_{11}^{(1)\alpha} \tag{3.74}$$
$$I_{22}^{(1)}(\mathbf{k}) = -\left[1-\alpha(\mathbf{k})\right]\left(\frac{1}{4} - \frac{1}{4}C_{11}^{(1)\alpha} + \frac{1}{2}C_{11}^{(2)\alpha} - 2C_{22}^{(1)}\right) \tag{3.75}$$

depends on the set of parameters

$$M = \langle S_z(i)\rangle = C_{11}^{(1)} - \frac{1}{2} = \left\langle S^+(i)S^-(i)\right\rangle - \frac{1}{2} \tag{3.76}$$
$$C_{11}^{(1)\alpha} = \left\langle S^{+\alpha}(i)S^-(i)\right\rangle \tag{3.77}$$
$$C_{11}^{(2)\alpha} = \langle S_z^\alpha(i)S_z(i)\rangle \tag{3.78}$$
$$C_{22}^{(1)} = -\left\langle l^+(i)l^-(i)\right\rangle. \tag{3.79}$$

These parameters are expressed in terms of the correlation function $C^{(m)}(i,j)$ and self-consistent equations are easily written by means of equations (3.58) and (3.59). However, in order to close the set of equations we need to know the zero-frequency constant

$$b_{11}^{(2)\alpha} = \frac{1}{3}\sum_{\mathbf{k}}\alpha(\mathbf{k})b_{11}^{(2)}(\mathbf{k}) = \frac{1}{2\pi}\frac{1}{3}\sum_{\mathbf{k}}\alpha(\mathbf{k})c_{11}^{(1,2)}(\mathbf{k}). \tag{3.80}$$

This quantity, undetermined within the bosonic sector, can be obtained, as proposed in Section 2, by fixing the representation of the GF by means of equation (2.19). In particular, the AC requires that

$$\left\langle S^+(i)l^-(i)\right\rangle = \frac{1}{2}M + \langle S_z^\alpha(i)S_z(i)\rangle + \frac{1}{2}\left\langle S^{+\alpha}(i)S^-(i)\right\rangle. \tag{3.81}$$

This equation, together with the others coming from the definitions (3.58) and (3.59), gives a set of five coupled self-consistent equation for the five parameters M, $C_{11}^{(1)\alpha}$, $C_{11}^{(2)\alpha}$, $C_{22}^{(1)}$, $b_{11}^{(2)\alpha}$. The system can be analytically solved. In particular, the magnetization per site M and the zero-frequency constant $b_{11}^{(2)}$ are given by

$$M = \frac{1}{6}\tanh\left(\frac{\beta h}{2}\right)\frac{2+3\cosh(\beta h)+\mathrm{e}^{\beta\frac{3}{2}J}}{\mathrm{e}^{\beta\frac{3}{2}J}+\cosh(\beta h)} \tag{3.82}$$
$$b_{11}^{(2)\alpha} = \frac{9\cosh(\beta h)-4-\mathrm{e}^{\beta\frac{3}{2}J}}{36\left[\mathrm{e}^{\beta\frac{3}{2}J}+\cosh(\beta h)\right]}. \tag{3.83}$$

It should be noted that other ZFC appear into the model. Again, they can be fixed by the Algebra Constraint. For example, the ZFC

$$b_{11}^{(2)} = \frac{1}{3}\sum_{\mathbf{k}}b_{11}^{(2)}(\mathbf{k}) = \frac{1}{2\pi}\frac{1}{3}\sum_{\mathbf{k}}c_{11}^{(1,2)}(\mathbf{k}) \tag{3.84}$$

is determined by means of the equation

$$\langle S_z(i)S_z(i)\rangle = \frac{1}{4} \tag{3.85}$$

and takes the value

$$b_{11}^{(2)} = \frac{9\cosh(\beta h)-4+5\mathrm{e}^{\beta\frac{3}{2}J}}{36\left[\mathrm{e}^{\beta\frac{3}{2}J}+\cosh(\beta h)\right]}. \tag{3.86}$$

We note that the two ZFC $b_{11}^{(2)\alpha}$ and $b_{11}^{(2)}$ assume the ergodic value M^2 only in the limit of very large external

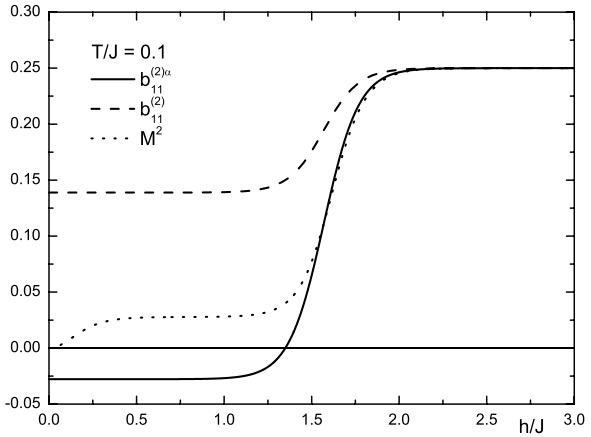

Fig. 3. The zero-frequency constants $b_{11}^{(2)\alpha}$ and $b_{11}^{(2)}$ are plotted as a function of the magnetic field for $T/J = 0.1$. For comparison, the ergodic value M^2 is also given.

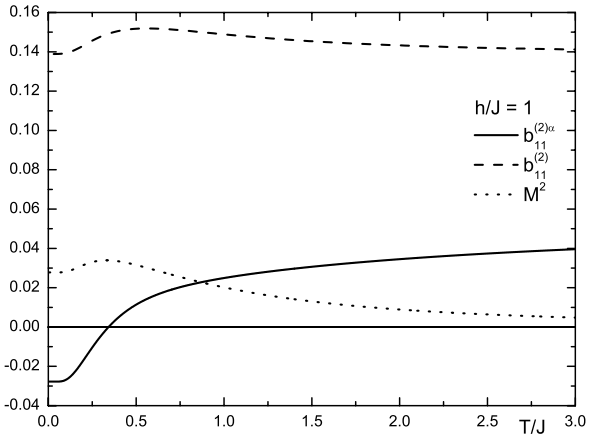

Fig. 4. The zero-frequency constant $b_{11}^{(2)\alpha}$ and $b_{11}^{(2)}$ are plotted as a function of the temperature for $h/J = 1$. For comparison, the ergodic value M^2 is also given.

magnetic field h. In Figures 3 and 4 the zero-frequency constants $b_{11}^{(2)\alpha}$ and $b_{11}^{(2)}$ are plotted as a function of the magnetic field h/J and temperature T/J, respectively. For comparison the ergodic value M^2 is also reported.

Let us now consider the $S^{\pm}$-channel (i.e., $m = 1$) and the relative *ZFC*. For $h \neq \frac{3}{2}J$ there are no zero-energy modes and the *ZFC* relative to the $S^{\pm}$-operators assume the ergodic value, i.e., zero. For the special case $h = \frac{3}{2}J$ a zero-energy mode $\omega_2^{(1)} = 0$ appears and the *ZFC* become nonergodic. Again, the Algebra Constraint can be used to fix these quantities. Straightforward calculations, according to the proposed scheme, give

$$b_{11}^{(1)} = \frac{1}{3}\sum_{\mathbf{k}} b_{11}^{(1)}(\mathbf{k}) = \frac{1}{2\pi}\frac{1}{3}\sum_{\mathbf{k}} c_{11}^{(2,1)}(\mathbf{k}) = \frac{3\mathrm{e}^{\beta\frac{3}{2}J}+4}{18\mathrm{e}^{-3\beta J}\left(1+\mathrm{e}^{\beta\frac{3}{2}J}\right)^3}$$

$$b_{11}^{(1)\alpha} = \frac{1}{3}\sum_{\mathbf{k}} \alpha(\mathbf{k}) b_{11}^{(1)}(\mathbf{k}) = \frac{1}{2\pi}\frac{1}{3}\sum_{\mathbf{k}} \alpha(\mathbf{k}) c_{11}^{(2,1)}(\mathbf{k}) = -\frac{3\mathrm{e}^{\beta\frac{3}{2}J}+1}{9\mathrm{e}^{-3\beta J}\left(1+\mathrm{e}^{\beta\frac{3}{2}J}\right)^3}.$$

Let us now consider the limit of zero temperature. From the previous expressions it is easy to derive the following.

- Case $J > 0$ (antiferromagnetic exchange)

$$M = \begin{cases} \frac{1}{2} & \text{for } h > \frac{3}{2}J \\ \frac{1}{6} & \text{for } h < \frac{3}{2}J \end{cases} \tag{3.87}$$

The two *ZFC* $b_{11}^{(2)\alpha}$ and $b_{11}^{(2)}$ take the values

$$b_{11}^{(2)} = b_{11}^{(2)\alpha} = \frac{1}{4} \qquad \text{for } h > \frac{3}{2}J \tag{3.88}$$

$$b_{11}^{(2)} = -5b_{11}^{(2)\alpha} = \frac{5}{36} \qquad \text{for } h < \frac{3}{2}J. \tag{3.89}$$

They are ergodic for $h > \frac{3}{2}J$ and nonergodic for $h < \frac{3}{2}J$. The other two *ZFC* $b_{11}^{(1)\alpha}$ and $b_{11}^{(1)}$ take the ergodic value (0) for any $h > 0$. In the limit of $h \to 0$ we obtain the ferromagnetic solution.

- Case $J < 0$ (ferromagnetic exchange)

$$M = \frac{1}{2}. \tag{3.90}$$

All the zero-frequency constants take the ergodic value. In the limit of $h \to 0$ we obtain again the ferromagnetic solution.

Let us now consider the case of absence of external magnetic field ($h = 0$). For this situation there are two energy modes, one in the S_z-channel (i.e., $m = 2$) $\omega_1^{(2)} = 0$ and one in the $S^{\pm}$-channel (i.e., $m = 1$) $\omega_1^{(1)} = 0$. In order to avoid divergencies in the correlation functions, it must be $\sigma^{(1,m)}(\mathbf{k}) = 0$ for $m = 1$, 2 and for all values of $\mathbf{k}$. It must be

$$I_{11}^{(m)}(\mathbf{k}) = 0 \Rightarrow M = 0 \tag{3.91}$$

$$I_{22}^{(m)}(\mathbf{k}) = 0 \Rightarrow 1 - C_{11}^{(1)\alpha} + 2C_{11}^{(2)\alpha} - 8C_{22}^{(1)} = 0. \tag{3.92}$$

By solving the self-consistent equations and by means of the Algebra Constraint, one finds the following nonergodic values for the *ZFC*:

$$b_{11}^{(2)} = \frac{1}{2}b_{11}^{(1)} = \frac{5}{36} \tag{3.93}$$

$$b_{11}^{(2)\alpha} = \frac{1}{2}b_{11}^{(1)\alpha} = \frac{5-\mathrm{e}^{\beta\frac{3}{2}J}}{36\left(\mathrm{e}^{\beta\frac{3}{2}J}+1\right)}. \tag{3.94}$$

At zero temperature

$$b_{11}^{(2)} = \frac{1}{2} b_{11}^{(1)} = \frac{5}{36} \tag{3.95}$$

$$b_{11}^{(2)\alpha} = \frac{1}{2} b_{11}^{(1)\alpha} = \begin{cases} -\dfrac{1}{36} & \text{for} J > 0 \\ \dfrac{5}{36} & \text{for} J < 0. \end{cases} \tag{3.96}$$

Summarizing, we have

T	h	J	M	S_z	$S^{\pm}$
0	$\to 0$	> 0	$\frac{1}{6}$	N	E
0	$\to 0$	< 0	$\frac{1}{2}$	E	E
$\to 0$	0	$\neq 0$	0	N	N
0	$\neq 0$	< 0	$\frac{1}{2}$	E	E
0	$< \frac{3}{2}J$	> 0	$\frac{1}{6}$	N	E
0	$> \frac{3}{2}J$	> 0	$\frac{1}{2}$	E	E
$\neq 0$	0	$\neq 0$	0	N	N
$\neq 0$	$\to \infty$	$\neq 0$	$\frac{1}{2}$	E	E
$\neq 0$	$\neq 0, \frac{3}{2}J$	$\neq 0$	$\neq 0$	N	E
$\neq 0$	$\frac{3}{2}J$	$\neq 0$	$\neq 0$	N	N

where E and N stays for an ergodic and nonergodic behavior of the corresponding *ZFC*, respectively. The first two lines of the table consider the cases in which we have a ferromagnetic solution.

The operator $S_z = \sum_{\mathbf{i}} S_z(i)$, as any constant of motion, has essentially a non ergodic dynamics. Actually, for high values of h/J, S_z is forced to assume the higher possible value $\frac{3}{2}$ and no fluctuations are allowed (i.e., the susceptibility vanishes): the dynamics returns to be ergodic. At zero temperature and for the ferromagnetic case (i.e., $J < 0$) the system is polarized and S_z is ergodic for all finite value of the magnetic field and in the ferromagnetic phase. The operator $S^+ = \sum_{\mathbf{i}} S^+(i)$ has an ergodic dynamics only in presence of the magnetic field h or in the ferromagnetic phase as it is no longer an integral of motion in these cases. Also, for the special case $h = \frac{3}{2}J$ the operator S^+ becomes nonergodic. These results show how the ergodicity of the dynamics of an operator can strongly depend on the boundary conditions.

It is worth noticing that the ferromagnetic phase has been obtained only at exactly zero temperature (i.e., when the applied magnetic field has been sent to zero after setting the temperature to zero). This is due to the size of the system; finite systems can sustain ordered phases only at exactly zero temperature. The correlation functions in direct space should be computed by finite sums over momenta (see Eq. (3.56)) and for vanishing spectra (e.g., for vanishing applied magnetic field; see Eq. (3.53)) the Bose factor (see the coth in Eq. (3.58)) diverges except at exactly zero temperature. Only in this latter case (i.e., $T = 0$) the corresponding spectral density function can retain a finite value (and consequently the magnetization too; see Eqs. (3.61, 3.64) and (3.72)) instead of being forced to vanish in order to avoid divergences in the direct space correlation functions. In practice, we allow the magnetization to be finite and search for a fully self-consistent solution. The system will self-adjust by selecting only those states with a finite magnetization of the same *sign* of that assigned as initial condition according to the ergodicity breaking inherent to any symmetry breaking.

We wish to remark that all the results obtained in this section exactly agree with those obtained by means of *ED*.

3.3 A narrow-band Bloch system in presence of an external magnetic field

A narrow-band Bloch system in presence of an external magnetic field is described by the following Hamiltonian

$$H = \sum_{\mathbf{ij}} (t_{\mathbf{ij}} - \mu\, \delta_{\mathbf{ij}})\, c^{\dagger}(i)\, c(j) - h \sum_{\mathbf{i}} n_3(i) \tag{3.97}$$

where $n_3(i)$ is the third component of the spin density operator and h is the intensity of the external magnetic field. The indices **i** and **j** run on an infinite d-dimensional lattice. Straightforward calculations show that the causal Green's function $G_C^{(\mu)}(i,j) = \langle \mathcal{T}\, [n_\mu(i)\, n_\mu(j)] \rangle$ and the correlation function $C^{(\mu)}(i,j) = \langle n_\mu(i)\, n_\mu(j) \rangle$ of the charge-spin operator $n_\mu(i) = c^{\dagger}(i)\, \sigma_\mu\, c(i)$ have the following expressions

$$G_C^{(\mu)}(\mathbf{k},\omega) = -\mathrm{i}\,(2\pi)^{d+1} a^{-d}\, \delta^{(d)}(k)\, \delta(\omega)\, \Gamma^{(\mu)} - Q^{(\mu)}(\mathbf{k},\omega) \tag{3.98}$$

$$C^{(\mu)}(\mathbf{k},\omega) = (2\pi)^{d+1}\, a^{-d}\, \delta^{(d)}(k)\, \delta(\omega)\, \Gamma^{(\mu)} + \left[1 + \tanh \frac{\beta\,\omega}{2}\right] \Im \left[Q^{(\mu)}(\, \mathbf{k},\omega) \right] \tag{3.99}$$

where $\delta^{(d)}(k)$ is the d-dimensional Dirac delta function. $Q^{(\mu)}(\mathbf{k},\omega)$ comes from the proper fermionic loop and is the Fourier transform of

$$Q^{(\mu)}(i,j) = \mathrm{Tr}\, [\sigma_\mu\, G_C(i,j)\, \sigma_\mu\, G_C(j,i)]\,. \tag{3.100}$$

Here $G_C(i,j) = \left\langle \mathcal{T}\, \left[c(i)\, c^{\dagger}(j)\right] \right\rangle$ is the causal fermionic function and has the expression

$$G_C(\mathbf{k},\omega) = \sum_{n=1}^{2} \frac{\sigma^{(n)}}{1 + e^{-\beta\, E_n(\mathbf{k})}} \times \left[\frac{1}{\omega - E_n(\mathbf{k}) + \mathrm{i}\delta} + \frac{e^{-\beta\, E_n(\mathbf{k})}}{\omega - E_n(\mathbf{k}) - \mathrm{i}\delta} \right] \tag{3.101}$$

with

$$E_1(\mathbf{k}) = -\mu - 2d\, t\, \alpha(\mathbf{k}) - h \tag{3.102}$$

$$E_2(\mathbf{k}) = -\mu - 2d\, t\, \alpha(\mathbf{k}) + h \tag{3.103}$$

$$\sigma^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \sigma^{(2)} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.104}$$

where

$$\alpha(\mathbf{k}) = \frac{1}{d} \sum_{i=1}^{d} \cos(k_i\, a). \tag{3.105}$$

The *ZFC* Γ^{μ} is fixed by the *AC* (2.19) which requires

$$\Gamma^{(\mu)} = \langle n_{\mu}(i)\, n_{\mu}(i)\rangle - \frac{a^d}{(2\pi)^{d+1}} \int d^d k\, d\omega \left[1 + \tanh\frac{\beta\,\omega}{2}\right] \Im\left[Q^{(\mu)}(\mathbf{k},\omega)\right]. \tag{3.106}$$

The loop $Q^{(\mu)}(\mathbf{k},\omega)$ can be calculated by means of (3.101). Calculations show

$$\frac{a^d}{(2\pi)^{d+1}} \int d^d k\, d\omega \left[1 + \tanh\frac{\beta\,\omega}{2}\right] \Im[Q^{(\mu)}(\mathbf{k},\omega)] = \langle n\rangle - \langle n_{\uparrow}\rangle^2 - \langle n_{\downarrow}\rangle^2 \quad for\ \ \mu = 0,3 \tag{3.107}$$

$$= \langle n\rangle - 2\,\langle n_{\uparrow}(i)\rangle\,\langle n_{\downarrow}(i)\rangle \quad for\ \ \mu = 1,2. \tag{3.108}$$

By recalling the *AC* (3.39), equation (3.106) gives for the *ZFC*

$$\Gamma^{(0)} = \langle n\rangle^2 \tag{3.109}$$

$$\Gamma^{(1,2)} = 0 \tag{3.110}$$

$$\Gamma^{(3)} = \langle n_3\rangle^2 \tag{3.111}$$

in accordance with the ergodic nature of the spin and charge dynamics in this system.

It is worth noting that the compressibility of this system can be computed by means of the general formula (2.18) that holds in the thermodynamic limit too and gives

$$\kappa = \frac{1}{\langle n\rangle^2}\frac{\beta}{2}\frac{a^d}{2(2\pi)^d}\sum_{n=1}^{2}\int d^d k \frac{1}{C_n(\mathbf{k})} \tag{3.112}$$

where $C_n(\mathbf{k}) = \cosh^2\left(\frac{\beta\,E_n(\mathbf{k})}{2}\right)$. We can see that an ergodic charge dynamics can lead to a non-ergodic value of the *ZFC* relative to the total number operator, which is an integral of motion. Also in the infinite systems the decoupling inspired by the requirement of ergodicity cannot always be applied.

3.4 The double exchange model

The Double Exchange Model is defined by the following Hamiltonian [34]

$$H = \sum_{\mathbf{ij}} (t_{\mathbf{ij}} - \mu\,\delta_{\mathbf{ij}})\, c^{\dagger}(i)\, c(j) - J_{\mathrm{H}} \sum_{\mathbf{i}} \vec{s}(i)\cdot\vec{S}(i) \tag{3.113}$$

$\vec{s}(i)$ is the spin density operator of the electron and is given by $\vec{s}(i) = \frac{1}{2} c^{\dagger}(i)\,\vec{\sigma}\,c(i)$; $\vec{S}(i)$ is a localized spin; J_{H} is the ferromagnetic Hund coupling ($J_{\mathrm{H}} > 0$). In the nearest-neighbor approximation for a d-dimensional cubic lattice with lattice constant a, $t_{\mathbf{ij}}$ takes the form

$$t_{\mathbf{ij}} = -2d\,t\,\alpha_{\mathbf{ij}} = -2d\,t\frac{1}{N}\sum_{\mathbf{k}} e^{\mathrm{i}\,\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}\,\alpha(\mathbf{k}) \tag{3.114}$$

where $\alpha(\mathbf{k})$ has been defined in the previous section and d is the dimensionality of the system. Let us introduce the Heisenberg field

$$B(i) = \begin{pmatrix} s^{+}(i) \\ S^{+}(i) \end{pmatrix} \tag{3.115}$$

where $s^{\pm}(i)$ and $S^{\pm}(i)$ are the standard rising and lowering spin operators.

This field satisfy the equation of motion

$$J(i) = \mathrm{i}\frac{\partial}{\partial t}B(i) = \begin{pmatrix} 2d\,t\,\rho(i) + J_{\mathrm{H}}\,\lambda(i) \\ -J_{\mathrm{H}}\,\lambda(i) \end{pmatrix} \tag{3.116}$$

where

$$\rho(i) = c_{\uparrow}^{\dagger\alpha}(i)\, c_{\downarrow}(i) - c_{\uparrow}^{\dagger}(i)\, c_{\downarrow}^{\alpha}(i) \tag{3.117}$$

$$\lambda(i) = s^{+}(i)\, S_z(i) - s_z(i)\, S^{+}(i). \tag{3.118}$$

We linearize the equation of motion (3.116) by projecting the source $J(i)$ on the basis (3.115)

$$J(i) \approx \sum_{\mathbf{j}} \varepsilon^{B}(\mathbf{i},\mathbf{j})\, B(\mathbf{j},t) \tag{3.119}$$

where the coefficients are determined by the following equation

$$\left\langle \left[J(\mathbf{i},t),\, B^{\dagger}(\mathbf{j},t)\right]\right\rangle = \sum_{\mathbf{l}} \varepsilon^{B}(\mathbf{i},\mathbf{l})\left\langle \left[B(\mathbf{l},t),\, B^{\dagger}(\mathbf{j},t)\right]\right\rangle. \tag{3.120}$$

Let us compute, within the framework described in Section 2, the causal Green's function

$$G(\mathbf{k},\omega) = \mathcal{F}\left\langle \mathcal{T}\left[B(i)\, B^{\dagger}(j)\right]\right\rangle = \sum_{n=1}^{2}\left[P\left(\frac{\sigma^{(n)}(\mathbf{k})}{\omega - \omega_n(\mathbf{k})}\right) - \mathrm{i}\,\pi\,\delta\left[\omega - \omega_n(\mathbf{k})\right] g^{(n)}(\mathbf{k})\right] \tag{3.121}$$

and the correlation function

$$C(\mathbf{k},\omega) = \mathcal{F}\left\langle B(i)\, B^{\dagger}(j)\right\rangle = \sum_{n=1}^{2}\delta\left[\omega - \omega_n(k)\right] c^{(n)}(\mathbf{k}) \tag{3.122}$$

$g^{(n)}(\mathbf{k})$ and $c^{(n)}(\mathbf{k})$ are still unknown functions; $\omega_n(\mathbf{k})$ are the eigenvalues of the matrix $\varepsilon^{B}(\mathbf{k})$; $\sigma^{(n)}(\mathbf{k})$ are the density spectral functions, completely determined by the matrices $\varepsilon^{B}(\mathbf{k})$ and $I^{B}(k) = \mathcal{F}\left\langle \left[B(i,t),\, B^{\dagger}(j,t)\right]\right\rangle$ by means of relation (2.8). We have

$$I^{B}(k) = \begin{pmatrix} 2\,\langle s_z(i)\rangle & 0 \\ 0 & 2\,\langle S_z(i)\rangle \end{pmatrix}. \tag{3.123}$$

For the sake of brevity, the explicit expressions for the energy matrix $\varepsilon^{B}(\mathbf{k})$, the energy spectra $\omega_n(\mathbf{k})$ and the spectral density functions $\sigma^{(n)}(\mathbf{k})$ are not reported here

and can be found in reference [35]. The calculations show that

$$\lim_{\mathbf{k}\to\mathbf{0}} \omega_2(\mathbf{k}) = 0 \tag{3.124}$$

$$\lim_{\mathbf{k}\to\mathbf{0}} \sigma^{(2)}(\mathbf{k}) = \frac{I^B_{11} I^B_{22}}{I^B_{11} + I^B_{22}} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \tag{3.125}$$

According to the scheme of calculation given in Section 2, we generally have

$$c^{(n)}(\mathbf{k}) = 2\pi\,\delta_{n2}\,\delta(\mathbf{k})\,\Gamma^B + \pi\left[1 + \coth\frac{\beta\omega_n(\mathbf{k})}{2}\right]\sigma^{(n)}(\mathbf{k}) \tag{3.126}$$

$$g^{(n)}(\mathbf{k}) = 2\delta_{n2}\,\delta(\mathbf{k})\,\Gamma^B + \coth\frac{\beta\omega_n(\mathbf{k})}{2}\sigma^{(n)}(\mathbf{k}). \tag{3.127}$$

The Green's functions have the following expressions

$$G(\mathbf{k},\omega) = -2\,\mathrm{i}\,\delta(\omega)\,\delta(\mathbf{k})\,\Gamma^B + \sum_{n=1}^{2} \frac{\sigma^{(n)}(\mathbf{k})}{1 - e^{-\beta\omega}}\left[\frac{1}{\omega - \omega_n(\mathbf{k}) + \mathrm{i}\,\delta} - \frac{e^{-\beta\,\omega}}{\omega - \omega_n(\mathbf{k}) - \mathrm{i}\,\delta}\right]$$

$$C(\mathbf{k},\omega) = 2\pi\,\delta(\omega)\,\delta(\mathbf{k})\,\Gamma^B + \pi\sum_{n=1}^{2}\delta\left[\omega - \omega_n(\mathbf{k})\right]\left[1 + \coth\frac{\beta\,\omega_n(\mathbf{k})}{2}\right]\sigma^{(n)}(\mathbf{k}).$$

The *ZFC* Γ^B is determined by means of the AC which requires

$$\frac{a^d}{(2\pi)^d}\Gamma^B = \left\langle B(i)\,B^\dagger(i)\right\rangle - \frac{a^d}{2(2\pi)^d}\sum_{n=1}^{2}\int d^dk\left[1 + \coth\frac{\beta\,\omega_n(\mathbf{k})}{2}\right]\sigma^{(n)}(\mathbf{k}). \tag{3.128}$$

In the case of a three-dimensional system the integral in equation (3.128) is finite. The Green's functions are fully determined and a ferromagnetic order does exist. In the case $d < 3$ we must distinguish two cases.

$T > 0$: In this case the divergence of the integrand in equation (3.128) is not integrable and the integral is divergent. The only physical solution is absence of ferromagnetic order. The magnetization must vanish

$$I^B_{11} = 2\,\langle s_z(i)\rangle = 0 \tag{3.129}$$

$$I^B_{22} = 2\,\langle S_z(i)\rangle = 0. \tag{3.130}$$

The spectral density function $\sigma^{(2)}(\mathbf{k})$ vanishes, in agreement with the general relation (2.12).

$T = 0$: In this case equation (3.128) becomes

$$\frac{a^d}{(2\pi)^d}\Gamma^B = \left\langle B(i)\,B^\dagger(i)\right\rangle - \frac{a^d}{(2\pi)^d}\sum_{n=1}^{2}\int d^dk\,\theta[\omega_n(\mathbf{k})]\,\sigma^{(n)}(\mathbf{k}) \tag{3.131}$$

where $\theta[\cdots]$ is the ordinary step function. We see that we can have ferromagnetic order for any dimension.

The results of the calculations for this model illustrate what stated in Section 2 regarding broken symmetry states in bulk systems. When a zero-energy mode appears in the ladder operator sector (e.g., S^+) the corresponding spectral density function, which is related to the order parameter (e.g., $\sigma \propto I \propto \langle S^z\rangle$), must vanish for all finite systems at finite temperatures and for all infinite systems when the divergence of the Fourier coefficients of the correlation function is not integrable in order to avoid divergences in the direct space correlation functions. At zero temperature it is always possible to have a finite value for the spectral density function and consequently for the order parameter. This result is a manifestation of the Mermin-Wagner theorem [21] which prevents the system from approaching, in some dimension, a particular ordered phase except at zero temperature.

4 Conclusions

In conclusion, the *GF* formalism for composite operators has been revised by making use of the equations of motion method. It has been shown that all the general relations (spectral representation, sum rules, etc.) can be derived without resorting to the knowledge of the complete set of eigenstates of the Hamiltonian. The advantage of using the equations of motion formalism is that it can be applied to any operatorial basis both exact and approximate. Special attention has been paid to the presence of the *ZFC* and to the problem of determining unknown parameters related to higher order correlators. The *ZFC* issue is quite relevant because such quantities are directly related to many response functions. We have shown that an effective and proper way to fix the representation is to impose the constraints coming from the AC and the *WT*. When these conditions are required, a set of self-consistent equations is obtained that permits to compute both the parameters appearing in the spectral functions and the zero-frequency component of the *GF*, avoiding the problem of *uncontrolled* and *uncontrollable* decouplings, which affects many different approximation schemes and has been here definitely solved.

Moreover, it is worth reminding the following issues, which have been discussed in detail all over the text:

- The two-time retarded (advanced) and causal bosonic *GF* carry substantially different information.
- The ergodicity condition cannot be used a priori to compute the *ZFC*.
- The Mermin-Wagner theorem [21] naturally appears as a requirement to avoid divergences in the direct space correlation functions.

It is also necessary pointing out – we already did it in Section 2 – that, although a careful choice of the components for the basic set makes possible the description of the main scales of energy present in the system under analysis, the inclusion of fully momentum and frequency

dependent self-energy corrections can be sometime necessary to take into account low-energy and virtual processes.

The calculation scheme has been illustrated by considering four systems: the two-site Hubbard model, the three site Heisenberg system, the narrow-band Bloch system and the Double-Exchange model. These examples clearly show the relevance and complexness of the above issues and illustrate in detail the application of the proposed procedure. It has been checked that the proposed scheme gives the exact result when solvable systems are considered.

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Appendix A: Generalized perturbative approach for SCES

Given a certain Hamiltonian $\hat{H} = \hat{H}\left[\varphi(i)\right]$, where $\varphi(i)$ denotes an Heisenberg electronic field $[i = (\mathbf{i}, t)]$ in spinorial notation satisfying canonical anticommutation relations, and a set of composite operators $\psi(i)$ chosen in the spirit of the discussion given in Section 1, the equations of motion for the propagator of the field $\psi(i)$ can be obtained by the dynamics obeyed by this latter which reads as

$$\mathrm{i}\frac{\partial}{\partial t}\psi(i) = [\psi(i), H] = J(i). \tag{A.1}$$

In complete generality, this equation can be rewritten as

$$\mathrm{i}\frac{\partial}{\partial t}\psi(i) = \sum_{\mathbf{j}} \varepsilon(\mathbf{i},\mathbf{j})\psi(\mathbf{j},t) + \delta J(i) \tag{A.2}$$

where the linear term $\varepsilon\,\psi$ represents the projection of the source $J(i)$ on the basis $\psi(i)$. The energy matrix $\varepsilon(\mathbf{i},\mathbf{j})$ can be computed by means of the equation

$$\left\langle \left[\delta J(\mathbf{i},t), \psi^{\dagger}(\mathbf{j},t)\right]_{\eta} \right\rangle = 0 \tag{A.3}$$

which defines the residual source $\delta J(i)$ and gives

$$\varepsilon(\mathbf{i},\mathbf{j}) = \sum_{\mathbf{l}} \left\langle \left[J(\mathbf{i},t), \psi^{\dagger}(\mathbf{l},t)\right]_{\eta} \right\rangle \left\langle \left[\psi(\mathbf{l},t), \psi^{\dagger}(\mathbf{j},t)\right]_{\eta} \right\rangle^{-1}. \tag{A.4}$$

Obviously, also less systematic projections of the source could be attempted and will result in different determinations of $\varepsilon(\mathbf{i},\mathbf{j})$ and $\delta J(i)$.

After equation (A.2), the Fourier transform $G_Q^{(\eta)}(\mathbf{k},\omega)$ of the *GF* $G_Q^{(\eta)}(i,j)$, where $Q = R$ (retarded), A (advanced), C (causal) (see definitions in Sect. 2), satisfies the following equation

$$G_Q^{(\eta)}(\mathbf{k},\omega) = G_{Q,0}^{(\eta)}(\mathbf{k},\omega) + G_{Q,0}^{(\eta)}(\mathbf{k},\omega)\left[I^{(\eta)}(\mathbf{k})\right]^{-1} \Sigma_Q^{(\eta)}(\mathbf{k},\omega) G_Q^{(\eta)}(\mathbf{k},\omega) \tag{A.5}$$

where the propagator $G_{Q,0}^{(\eta)}(\mathbf{k},\omega)$ is defined by the equation

$$[\omega - \varepsilon(\mathbf{k})]\, G_{Q,0}^{(\eta)}(\mathbf{k},\omega) = I^{(\eta)}(\mathbf{k}). \tag{A.6}$$

The matrix $I^{(\eta)}(\mathbf{k})$, known as the normalization matrix, is defined as

$$I^{(\eta)}(\mathbf{k}) = \mathcal{F}\left\langle \left[\psi(\mathbf{i},t), \psi^{\dagger}(\mathbf{j},t)\right]_{\eta} \right\rangle \tag{A.7}$$

$\Sigma_Q^{(\eta)}(\mathbf{k},\omega)$ is the proper self-energy and has the expression

$$\Sigma_Q^{(\eta)}(\mathbf{k},\omega) = B_{Q,irr}^{(\eta)}(\mathbf{k},\omega) I^{(\eta)}(\mathbf{k})^{-1} \tag{A.8}$$

where $B_{Q,irr}^{(\eta)}(\mathbf{k},\omega)$ is the irreducible part of the propagator $B_Q^{(\eta)}(\mathbf{k},\omega) = \mathcal{F}\left\langle \mathcal{Q}\left[\delta J(i)\delta J^{\dagger}(j)\right]\right\rangle$. Equation (A.5) can be formally solved to give

$$G_Q^{(\eta)}(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon(\mathbf{k}) - \Sigma_Q^{(\eta)}(\mathbf{k},\omega)} I^{(\eta)}(\mathbf{k}). \tag{A.9}$$

Equations (A.5) and (A.9) are nothing else than the Dyson equation for a formulation based on composite fields and represents the starting point for a perturbative calculation in terms of the propagator $G_{Q,0}^{(\eta)}(\mathbf{k},\omega)$. The properties and the determination of this latter are derived and discussed in Section 2.

Appendix B: KMS relation and the general formulation

From the definitions (2.1–2.3) we can derive the following exact relations

$$G_R^{(\eta)}(i,j) + G_A^{(\eta)}(i,j) = 2G_C^{(\eta)}(i,j) - \left\langle \left[\psi(i),\, \psi^{\dagger}(j)\right]_{-\eta} \right\rangle \tag{B.1a}$$

$$G_R^{(\eta)}(i,j) - G_A^{(\eta)}(i,j) = \left\langle \left[\psi(i),\, \psi^{\dagger}(j)\right]_{\eta} \right\rangle. \tag{B.1b}$$

By making use of the Kubo-Martin-Schwinger (*KMS*) relation $\langle A(t)\, B(t')\rangle = \langle B(t')\, A(t + \mathrm{i}\,\beta)\rangle$, where $A(t)$ and $B(t)$ are Heisenberg operators at time t, the η-commutator can be expressed in terms of the correlation function as

$$\left\langle \left[\psi(i),\, \psi^{\dagger}(j)\right]_{\eta} \right\rangle = \frac{1}{M}\sum_{\mathbf{k}} \frac{1}{2\pi}\int d\omega\, e^{\mathrm{i}\ \mathbf{k}\cdot(\mathbf{i}-\mathbf{j}) - \mathrm{i}\,\omega(t_i - t_j)} \times \left[1 + \eta\, e^{-\beta\,\omega}\right] C(\mathbf{k},\omega) \tag{B.2}$$

where M is the number of sites and $\mathbf{k}$ runs over the first Brillouin zone. Then, the equations (B.1) in momentum space become

$$\sum_{l=1}^{n} \delta[\omega - \omega_l(\mathbf{k})] \left\{ g_C^{(\eta,l)}(\mathbf{k}) - \frac{1}{2\pi} \left[1 - \eta\, e^{-\beta\,\omega}\right]\, c^{(l)}(\mathbf{k}) \right\} = 0 \quad \text{(B.3a)}$$

$$\sum_{l=1}^{n} \delta[\omega - \omega_l(\mathbf{k})] \left\{ \sigma^{(\eta,l)}(\mathbf{k}) - \frac{1}{2\pi} \left[1 + \eta\, e^{-\beta\,\omega}\right]\, c^{(l)}(\mathbf{k}) \right\} = 0. \quad \text{(B.3b)}$$

In order to solve these equations, we have to take into account that for any given momentum $\mathbf{k}$ we can always write

$$\omega_l(\mathbf{k}) = \begin{cases} = 0 & \text{for } l \in \mathcal{A}(\mathbf{k}) \subseteq \aleph = \{1, \ldots, n\} \\ \neq 0 & \text{for } l \in \mathcal{B}(\mathbf{k}) = \aleph - \mathcal{A}(\mathbf{k}). \end{cases} \quad \text{(B.4)}$$

Obviously, $\mathcal{A}(\mathbf{k})$ can also be the empty set (i.e., $\mathcal{A}(\mathbf{k}) = \emptyset$ and $\mathcal{B}(\mathbf{k}) = \aleph$). Combined use of equations (B.3) and (B.4) gives the results reported in Section 2 (Eq. (2.10)).

Appendix C: Formulation in the limit of zero temperature

At zero temperature equation (B.3) is not applicable and we should proceed in the following way (the usual derivation in terms of a complete set of eigenstates of the Hamiltonian can be found in Ref. [36]).

Let us consider the correlation functions

$$C_{\psi\psi^\dagger}(i,j) = \left\langle \psi(i)\psi^\dagger(j) \right\rangle = \frac{1}{N} \sum_k \frac{1}{2\pi} \int d\omega\, e^{\mathrm{i}[\mathbf{k}\cdot(\mathbf{i}-\mathbf{j}) - \omega(t_i - t_j)]} C_{\psi\psi^\dagger}(\mathbf{k},\omega)$$

$$C_{\psi^\dagger\psi}(i,j) = \left\langle \psi^\dagger(i)\psi(j) \right\rangle = \frac{1}{N} \sum_k \frac{1}{2\pi} \int d\omega\, e^{\mathrm{i}[\mathbf{k}\cdot(\mathbf{i}-\mathbf{j}) - \omega(t_i - t_j)]} C_{\psi^\dagger\psi}(\mathbf{k},\omega).$$

By taking the limit $T \longrightarrow 0$ of the *KMS* relation

$$C_{\psi^\dagger\psi}(\mathbf{k},\omega) = e^{-\beta\omega} C_{\psi\psi^\dagger}(\mathbf{k},\omega) \quad \text{(C.1)}$$

it is immediate to see that for any finite value of the Fourier coefficients, it must be

$$C_{\psi\psi^\dagger}(\mathbf{k},\omega) = \begin{cases} \neq 0 & \text{for } \omega \geq 0 \\ = 0 & \text{for } \omega < 0 \end{cases} \quad \text{(C.2)}$$

$$C_{\psi^\dagger\psi}(\mathbf{k},\omega) = \begin{cases} = 0 & \text{for } \omega > 0 \\ \neq 0 & \text{for } \omega \leq 0. \end{cases} \quad \text{(C.3)}$$

Furthermore

$$C_{\psi^\dagger\psi}(\mathbf{k},0) = C_{\psi\psi^\dagger}(\mathbf{k},0). \quad \text{(C.4)}$$

Let us consider the energy spectra $\omega_l(\mathbf{k})$ and let us write in complete generality, for any given momentum $\mathbf{k}$

$$\omega_l(\mathbf{k}) = \begin{cases} = 0 \text{ for } l \in \mathcal{A}(\mathbf{k}) \subseteq \aleph \\ > 0 \text{ for } l \in \mathcal{C}(\mathbf{k}) \subseteq \aleph \\ < 0 \text{ for } l \in \mathcal{D}(\mathbf{k}) \subseteq \aleph. \end{cases} \quad \text{(C.5)}$$

Then, equations (B.1) in momentum space are written as

$$\delta(\omega) \sum_{l\in\mathcal{A}(\mathbf{k})} \left\{ g_C^{(\eta,l)}(\mathbf{k}) - \frac{1}{2\pi}\,(1-\eta)\, c^{(l)}_{\psi\psi^\dagger}(\mathbf{k}) \right\} + \sum_{l\in\mathcal{C}(\mathbf{k})} \delta[\omega - \omega_l(\mathbf{k})] \left\{ g_C^{(\eta,l)}(\mathbf{k}) - \frac{1}{2\pi} c^{(l)}_{\psi\psi^\dagger}(\mathbf{k}) \right\} + \sum_{l\in\mathcal{D}(\mathbf{k})} \delta[\omega - \omega_l(\mathbf{k})] \left\{ g_C^{(\eta,l)}(\mathbf{k}) + \frac{\eta}{2\pi} c^{(l)}_{\psi^\dagger\psi}(\mathbf{k}) \right\} = 0 \quad \text{(C.6a)}$$

$$\sum_{l=1}^{n} \delta[\omega - \omega_l(\mathbf{k})] \left\{ \sigma^{(\eta,l)}(\mathbf{k}) - \frac{1}{2\pi}\,(1+\eta)\, c^{(l)}_{\psi\psi^\dagger}(\mathbf{k}) \right\} + \sum_{l=1}^{n} \delta[\omega - \omega_l(\mathbf{k})] \left\{ \sigma^{(\eta,l)}(\mathbf{k}) - \frac{1}{2\pi} c^{(l)}_{\psi\psi^\dagger}(\mathbf{k}) \right\} + \sum_{l=1}^{n} \delta[\omega - \omega_l(\mathbf{k})] \left\{ \sigma^{(\eta,l)}(\mathbf{k}) - \frac{\eta}{2\pi} c^{(l)}_{\psi^\dagger\psi}(\mathbf{k}) \right\} = 0. \quad \text{(C.6b)}$$

The solution of these equations gives the following expressions for the *GF*

$$G^{(\eta)}_{R,A}(\mathbf{k},\omega) = \sum_{l\in\aleph} \frac{\sigma^{(\eta,l)}(\mathbf{k})}{\omega - \omega_l(\mathbf{k}) \pm \mathrm{i}\,\delta} \quad \text{(C.7a)}$$

$$G^{(\eta)}_C(\mathbf{k},\omega) = \Gamma(\mathbf{k}) \left(\frac{1}{\omega + \mathrm{i}\,\delta} + \frac{\eta}{\omega - \mathrm{i}\,\delta} \right) + \sum_{l\notin\mathcal{A}(\mathbf{k})} \sigma^{(\eta,l)}(\mathbf{k}) \left[\frac{\theta[\omega_l(\mathbf{k})]}{\omega - \omega_l(\mathbf{k}) + \mathrm{i}\,\delta} + \frac{\theta[-\omega_l(\mathbf{k})]}{\omega - \omega_l(\mathbf{k}) - \mathrm{i}\,\delta} \right] \quad \text{(C.7b)}$$

$$C_{\psi\psi^\dagger}(\mathbf{k},\omega) = 2\pi\,\delta(\omega)\,\Gamma(\mathbf{k}) + 2\pi \sum_{l\notin\mathcal{A}(\mathbf{k})} \delta[\omega - \omega_l(\mathbf{k})]\,\theta[\omega_l(\mathbf{k})]\,\sigma^{(\eta,l)}(\mathbf{k}) \quad \text{(C.7c)}$$

$$C_{\psi^\dagger\psi}(\mathbf{k},\omega) = 2\pi\,\delta(\omega)\,\Gamma(\mathbf{k}) + 2\pi\eta \sum_{l\notin\mathcal{A}(\mathbf{k})} \delta[\omega - \omega_l(\mathbf{k})]\,\theta[-\omega_l(\mathbf{k})]\,\sigma^{(\eta,l)}(\mathbf{k}). \quad \text{(C.7d)}$$

It is fairly easy to check that these expressions (C.7) correspond to limit $T \to 0$ ($\beta \to \infty$) of the expressions (2.13).

Appendix D: Useful relations

We note the dispersion relations

$$\Re\left[G^{(\eta)}_{R,A}(\mathbf{k},\omega)\right] = \mp\frac{1}{\pi}\mathcal{P}\left\{\int d\omega' \frac{1}{\omega-\omega'}\Im\left[G^{(\eta)}_{R,A}(\mathbf{k},\omega')\right]\right\} \quad \text{(D.1a)}$$

$$\Re\left[G^{(\eta)}_{C}(\mathbf{k},\omega)\right] = -\frac{1}{\pi}\mathcal{P}\left\{\int d\omega' \frac{1}{\omega-\omega'}\frac{1+\eta\, e^{-\beta\,\omega'}}{1-\eta\, e^{-\beta\,\omega'}}\Im\left[G^{(\eta)}_{C}(\mathbf{k},\omega')\right]\right\}. \quad \text{(D.1b)}$$

This latter relation is valid for causal *fermionic GF* (i.e., for $\eta = 1$) only when $\Gamma(\mathbf{k}) = 0$.

For the retarded and advanced *GF*, which are analytical functions satisfying the standard Kramers-Kronig relations (D.1a), we can establish a spectral representation

$$G^{(\eta)}_{R,A}(\mathbf{k},\omega) = \int d\omega' \frac{\rho^{(\eta)}(\mathbf{k},\omega')}{\omega-\omega'\pm \mathrm{i}\,\delta} \quad \text{(D.2)}$$

where we introduced the spectral function

$$\rho^{(\eta)}(\mathbf{k},\omega) = \sum_{l=1}^{n}\delta[\omega-\omega_l(\mathbf{k})]\,\sigma^{(\eta,l)}(\mathbf{k}) = \mp\frac{1}{\pi}\Im\left[G^{(\eta)}_{R,A}(\mathbf{k},\omega)\right]. \quad \text{(D.3)}$$

A spectral representation for the causal *GF* can be established in the following form

$$G^{(\eta)}_{C}(\mathbf{k},\omega) = \int d\omega' \frac{\rho^{(\eta)}(\mathbf{k},\omega')}{1+\eta\, e^{-\beta\,\omega'}}\left(\frac{1}{\omega-\omega'+\mathrm{i}\,\delta}+\frac{\eta\, e^{-\beta\,\omega'}}{\omega-\omega'-\mathrm{i}\,\delta}\right). \quad \text{(D.4)}$$

This latter relation is valid for causal *bosonic GF* (i.e., for $\eta = -1$) only when $\Gamma(\mathbf{k}) = 0$.

We also note the sum rule

$$\int d\omega\, \rho^{(\eta)}(\mathbf{k},\omega) = \sum_{l=1}^{n}\sigma^{(\eta,l)}(\mathbf{k}) = I^{(\eta)}(\mathbf{k}). \quad \text{(D.5)}$$

This is a particular case of the general sum rule

$$\int d\omega\,\omega^p\,\rho^{(\eta)}(\mathbf{k},\omega) = \sum_{l=1}^{n}\omega_l^p(\mathbf{k})\,\sigma^{(\eta,l)}(\mathbf{k}) = M^{(\eta,p)}(\mathbf{k}) = \varepsilon^p\, I \quad \text{(D.6)}$$

where $M^{(\eta,p)}(\mathbf{k})$ are the spectral moments

$$M^{(\eta,p)}(\mathbf{k}) = \mathcal{F}\left[\mathrm{i}\frac{\partial^p}{\partial\, t_i^p}\left\langle[\psi(i),\,\psi(j)]_\eta\right\rangle\right]_{t_i=t_j} \quad \text{(D.7)}$$

and the last equality in equation (D.6) holds only when equation (1.2) also does.

Finally, by exploiting the independence of $c^{(l)}(\mathbf{k})$ on η (see Eq. (2.10c)), we have

$$\sigma^{(-1,l)}(\mathbf{k}) = \tanh\frac{\beta\,\omega_l(\mathbf{k})}{2}\sigma^{(1,l)}(\mathbf{k}) \quad \forall l\in\mathcal{B}(\mathbf{k}). \quad \text{(D.8)}$$

In absence of symmetry breaking, equations (2.12) and (D.8), together with equation (2.8), give

$$I^{(-1)}_{\alpha\beta}(\mathbf{k}) = \sum_{l\delta}\Omega_{\alpha l}(\mathbf{k})\tanh\frac{\beta\,\omega_l(\mathbf{k})}{2}\Omega^{-1}_{l\delta}(\mathbf{k})\,I^{(1)}_{\delta\beta}(\mathbf{k}). \quad \text{(D.9)}$$

The independence of $C(\mathbf{k},\omega)$ on η (see Eq. (2.14)) gives

$$\Im\left[G^{(\eta)}_{C}(\mathbf{k},\omega)\right] = \Im\left[G^{(-\eta)}_{R}(\mathbf{k},\omega)\right]. \quad \text{(D.10)}$$

In terms of spectral densities

$$\sum_{l\in\mathcal{A}(\mathbf{k})}\delta[\omega-\omega_l(\mathbf{k})]\left[\frac{\sigma^{(1,l)}(\mathbf{k})}{1+e^{-\beta\,\omega_l(\mathbf{k})}}-\frac{\sigma^{(-1,l)}(\mathbf{k})}{1-e^{-\beta\,\omega_l(\mathbf{k})}}\right]=0. \quad \text{(D.11)}$$

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