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Strongly Correlated Electron Systems: An Operatorial Perspective

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ABSTRACT

We discuss the operatorial approach to the study of strongly correlated electron systems and show how the exact solution of target models on small clusters chosen ad-hoc (minimal models) can suggest very efficient bulk approximations. We use the Hubbard model as case study (target model) and we analyze and discuss the crucial role of spin fluctuations in its 2-site realization (minimal model). Accordingly, we devise a novel three-pole approximation for the 2D case, including in the basic field an operator describing the dressing of the electronic one by the nearest-neighbor spin-fluctuations. Such a solution is in very good agreement with the exact one in the minimal model (2-site case) and performs very well once compared to advanced (semi-)numerical methods in the 2D case, being by far less computational-resource demanding.

1. Introduction

Strongly correlated systems remain one of the most stimulating intellectual challenges in modern condensed matter theory [1–10] and solid state physics [11–14]. In this short paper we show the capabilities of the operatorial approach, based on the equations of motion and the Green's function formalisms [15–22] to very efficiently handle a generic strongly correlated electron system reaching a deep and rich understanding of its unconventional properties. We characterize the exact solution of a generic interacting fermionic Hamiltonian and discuss how such an analysis effectively performed on the smallest cluster where all Hamiltonian terms result *active* (the minimal model) can suggest very efficient and controlled approximation schemes for the corresponding bulk system, which remains the final target of the analysis.

Then, we use the 2D Hubbard model as case study, and, according to the general recipe, we study the exact solution of its two-site version (the corresponding minimal model) to capture the necessary ingredients to devise a novel and efficient three-pole (3p) bulk approximation. As the spin fluctuations prove to play a crucial role, we enrich the standard two-pole (2p) operatorial basis, formed by the two Hubbard operators [18,21,22,24–26], with a third operator describing the electronic one dressed by the nearest-neighbor spin fluctuations. This 3p approximation is in very good agreement with the exact solution obtained in the two-site case (the minimal model) and performs very well with respect to advanced (semi-)numerical methods [27] in the 2D case (the target model), being by far less computational-resource demanding and, in principle, more accurate in frequency and momentum resolution. Moreover, this route, by treating spin fluctuations with extreme care and by improving the momentum selectivity of the spectral properties, opens up the possibility to directly address photoemission results of strongly correlated materials on a level before possible only including explicitly a residual self-energy in the calculations [28].

2. The operatorial approach

We consider a system of electrons described by a Hamiltonian H in terms of canonical fermionic operators $c_\lambda(r)$, in the Heisenberg picture [$r = (\mathbf{r}, t)$, being $\mathbf{r}$ the position and t the time], where the index λ identifies the quantum state. We aim to evaluate the generic observable $A = \langle \widehat{A}[\{c_\lambda(r)\}]\rangle$ where $\langle\ldots\rangle$ denotes the quantum-statistical average in the grand-canonical ensemble and $\widehat{A}[\{c_\lambda(r)\}]$ stands for a generic operator, which can be always expressed in terms of a *string* of c-operators without any loss of generality. If we split this *string* into two sub-*strings*, we can consider any observable as the correlation function C of two composite operators (COs) ψ and φ, which are expressed in terms of the two sub-*strings* of c-operators identified by the splitting: $A = C = \langle \psi\phi^\dagger\rangle$. Once all the relevant COs have been individuated according to all the A – and the corresponding C – actively under analysis, we consider the retarded Green's function (GF) of such COs (in matricial notation): $G(t - t') = \langle \mathcal{R}[\Psi(t)\Psi^\dagger(t')]\rangle$, where Ψ is a vector hosting all relevant COs and is dubbed operatorial *basis*. In order to compute $G(t - t')$, we need to solve the corresponding Dyson equation, which is generated by time-differentiation. Accordingly, we need the equations of motion of all relevant COs and, therefore, of Ψ. In

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principle, by adding in Ψ all COs appearing in turn in the current J (the vector of COs obtained by time-differentiation, that is by the commutation with H, of Ψ) of the components of Ψ, one can close the hierarchy of equations of motion and obtain an exact expression for G:

$$J = i\frac{\partial}{\partial t}\Psi = [\Psi, H] = \varepsilon\Psi \tag{1}$$

$$i\frac{\partial}{\partial t}G(t) = i\delta(t)I + \varepsilon G(t) \Rightarrow G(\omega) = \frac{1}{\omega - \varepsilon}I \tag{2}$$

ε is dubbed the *energy* matrix, whose elements are expressed only in terms of the Hamiltonian parameters, and $I = \langle\{\Psi, \Psi^\dagger\}\rangle$ is dubbed the *normalization* matrix, whose elements are correlation functions. Such correlations functions can be either correlation functions of elements of Ψ, and can therefore be computed self-consistently, or they become unknowns of the theory. There are two possible routes to compute exactly such unknowns: (a) to include in Ψ all COs necessary to compute them self-consistently and all COs appearing in the related currents, and repeat this procedure (re-computing I) as many times as it would be necessary; (b) to use the constraints coming from the non-canonical algebra closed by the COs in Ψ [Algebra Constraints (ACs)] or from the symmetries enjoyed by the system (e.g. Ward-Takahashi identities) to compute the unknowns again self-consistently. The second route leads to an operatorial *basis* Ψ with a minor number of components and it is therefore preferable in terms of simplicity of the calculations, although the first route usually leads to a more profound understanding of the system under analysis.

There is a special operatorial *basis* Ψ, the *essential* basis, that is the one containing all $c_\lambda(r)$ or COs that can give all of them in sum, together with all COs necessary to compute the elements of the related I self-consistently through one of the two routes reported above. Computing the Green's function G of the essential basis corresponds to find the exact solution of the system as one knows all possible electronic Green's functions of the system. In such a case, the eigenvalues of the *energy* matrix ε are the fundamental excitations of the system and the COs, identified by its eigenvalues, the new quasi-particles appearing in the system because of the interactions present in the Hamiltonian H. This is the best result one can get as (i) it is expressed in terms of transition energies and COs identifying the relevant electronic transitions in the system, that is the new non-interacting quasi-particles, which is the way we naturally thinks about an interacting system; (ii) the information contained in the solution can be easily scaled between different cluster sizes and spatial dimensions. Moreover, starting from COs representing the physical degrees of freedom of the system (charge, spin, pair, ... fluctuations dressing the electronic transitions), one can also investigate the relevance each of them has with respect to the physics of the system under analysis. As a matter of fact, the diagonal entries of the normalization matrix I give a measure of the *weight* of any CO (it is just 1 for any $c_\lambda(r)$) as a function of the Hamiltonian and the external parameters (temperature, pressure, ...), while its off-diagonal entries give a measure of the degree of orthogonality (it is just 0 for any couple of distinct $c_\lambda(r)$), that is of *independence*, between two distinct COs.

Obviously, such recipe can be used just as it has been given above only if the system under analysis has only a small number of degrees of freedom or if just few (or none) of them interact. In these cases, the number of COs in the essential basis is small enough to find the exact solution of the system (e.g., a non-interacting system will just have all and only the $c_\lambda(r)$ in Ψ). In all other cases, some approximations have to be employed. Fundamentally, one can decide to include only a certain number of selected COs in the essential basis Ψ according to his own physical intuition (see below) and project the current of this Ψ on Ψ itself

$$J = i\frac{\partial}{\partial t}\Psi = \varepsilon\Psi + \delta J \tag{3}$$

$$\varepsilon = \langle\{J, \Psi^\dagger\}\rangle I^{-1} \tag{4}$$

Then, one has the choice either to neglect the *residual* current δJ (leading to a pole approximation) or to compute according to any of the available approximations in the literature (e.g., NCA, IPT, ...) [9] the related *residual* self-energy $\Sigma(t - t') = \langle\mathcal{R}[\delta J(t)\delta J^\dagger(t')]\rangle$ leading to a full-fledge expression for G [28]: $G = \frac{1}{\omega - \varepsilon - \Sigma}I$. Once this has been done, one is left with the computation of the correlation functions appearing now both in ε and I. The first route (a) is obviously not available (*i.e.* the number of COs in Ψ has been fixed) and one can only use the second one (b) (e.g. exploiting the ACs dictated by the choice of Ψ) and compute the remaining correlation functions, if any – ACs can be just enough [21] or even exceed the needs – by means of any of the available approximations in the literature and, in particular, the *operatorial projection* [23]: $\Phi \cong \langle\{\Phi, \Psi^\dagger\}\rangle I^{-1}\Psi$. This latter procedure has to be preferred to any other as it is actually what has already been used to approximate the current J in Eqs. (3) and (4): J has been split into its projection on the basis Ψ ($\varepsilon\Psi$) and into the residual current δJ, this latter describing a physics that is *orthogonal* to the one described by the *carefully* chosen basis Ψ. Any *unknown* correlation function can always be computed, although in an approximate way, by splitting its averaged string of $c_\lambda(r)$ into two COs (this makes the procedure not unique and the physical intuition again plays a major role in this choice), one of which belonging to Ψ – this is always possible as all $c_\lambda(r)$ should anyway belong to Ψ – and projecting the other CO over the basis Ψ [23].

Let us come finally to the choice of the COs to employ in the approximate essential basis Ψ. Among the many possible recipes [29] (e.g., the essential basis of the Hamiltonian reduced just to the relevant interaction term, the first operators appearing in the equations of motion hierarchy of the canonical electronic operators of the system, ...), the exact essential basis for the smallest cluster where all Hamiltonian terms result *active* (the minimal model) seems to be the best choice as it assures that all relevant energy scales in the system are taken into account together with all quasi-particles generated by the interactions. Moreover, such a choice allows to re-use the exact results obtained on such minimal cluster to devise very efficient and controlled bulk approximations, which is the main aim of the whole described procedure and of the operatorial approach overall. This benefit does not only counterbalance, but greatly overcomes the greater efforts necessary to get the exact solution on small clusters in the operatorial approach with respect to ordinary exact diagonalization, whose results cannot be re-used at all on larger and larger clusters, and definitely not for the bulk.

3. Case study: the two-dimensional Hubbard model

As relevant case study for the application of the operatorial approach, we study the paramagnetic solution of the single-band Hubbard model on the square lattice described by the Hamiltonian

$$H = \sum_{\mathbf{i}} \left(-4t\vec{c}^\dagger(i)\cdot\vec{c}^{\,\alpha}(i) + Un_\uparrow(i)n_\downarrow(i) - \mu n(i)\right) \tag{5}$$

where $c(i)$ is the Heisenberg electronic field operator in spinorial notation, $n_\sigma(i) = c_\sigma^\dagger(i)c_\sigma(i)$ and $n(i) = \sum_\sigma n_\sigma(i)$ are the number per spin and total number operator, respectively, $\cdot$ is the internal product in spin space, and $\vec{c}^{\,\alpha}(i) = \sum_{\mathbf{j}}\alpha_{\mathbf{ij}}\vec{c}(\mathbf{j}, t)$ where $\alpha_{\mathbf{ij}} = \frac{1}{4}\delta_{\langle\mathbf{ij}\rangle}$ is the nearest neighbor ($\langle\mathbf{ij}\rangle$) projector. t is the nearest-neighbor hopping integral, U the local Coulomb repulsion, and μ the chemical potential. Hereafter, all energies are expressed in units of t.

3.1. Two-site exact solution

For the two-site Hubbard model all possible correlation functions can be computed and all COs equation of motion hierarchies can be closed by means of the following exact essential basis Ψ:

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