The 2-site Hubbard and t-J models

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Received 16 July 2003
Published online 30 January 2004 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2004

Abstract. The fermionic and bosonic sectors of the 2-site Hubbard model have been exactly solved by
means of the equation of motion and Green’s function formalism. The exact solution of the t-J model has
been also reported to investigate the low-energy dynamics. We have successfully searched for the exact
eigenoperators, and the corresponding eigenenergies, having in mind the possibility to use them as an
operational basis on the lattice. Many local, single-particle, thermodynamical and response properties have
been studied as functions of the external parameters and compared between the two models and with some
numerical and exact results. It has been shown that the 2-site Hubbard model already contains the most
relevant energy scales of the Hubbard model: the local Coulomb interaction \( U \) and the spin-exchange one
\( J = \frac{4t^2}{U} \). As a consequence of this, for some relevant properties (kinetic energy, double occupancy, energy,
specific heat and entropy) and as regards the metal-insulator transition issue, it has resulted possible
to almost exactly mime the behavior of larger systems, sometimes using a higher temperature to get a
comparable level spacing. The 2-site models have been also used as toy models to test the efficiency of
the Green’s function formalism for composite operators. The capability to reproduce the exact solutions,
obtained by the exact diagonalization technique, gives a firm ground to the approximate treatments based
on this formalism.

PACS. 71.10.-w Theories and models of many-electron systems – 71.10.Fd Lattice fermion models
(Hubbard model, etc.)

1 Introduction

Two are the aspects that gave so much popularity to the Hubbard model: the richness of its dynamics that is
thought to permit a description of many puzzling issues like metal-insulator transition, itinerant magnetism, elec-
tronic superconductivity, and the simplicity of the Hamiltonian structure that let one speculate about the possi-
bility of finding the exact and complete solution for any realization of the underlying lattice. Anyway, although the
model has been studied more than any other one in the last fifty years, very few exact results are available and what
we have mainly regards either finite clusters or the infinite chain (i.e., the 1D case). For finite clusters of 2 \([1,2]\) or
4 \([2–6]\) sites it is possible to find the complete set of eigenstates and eigenvalues of the Hamiltonian and compute
any quantity by means of the thermal averages. However, it is not easy at all, although possible in principle, to ex-
tract valuable and scalable (i.e., which can be used to find the solutions of bigger and bigger clusters and, ulti-
mately, of the infinite lattice cases) information regarding the effective excitations present in the system, the opera-
tors describing them and their dynamics. For the infinite chain neither, we have all the information we wish; the

Bethe ansatz is a very powerful tool, but is severely limited as regards the range of applicability of the self-consistent
equations it supplies and the quantities for which it gives an answer.

In this manuscript, in order to overcome the limitations discussed above, we have exactly solved the Hubbard
model, on a 2-site cluster, completely within the equations of motion and the Green’s function formalism. By using
this approach, we have had the possibility to find the complete set of eigenoperators of the Hamiltonian and the cor-
responding eigenenergies. This information has been really fundamental as it permitted a deeper comprehension of
the features shown by the properties we have analyzed. It is worth noting that the Hubbard model on a 2-site
cluster is the smallest system where both terms of the Hamiltonian (i.e., kinetic and electrostatic) are effective
and contributes to the dynamics.

By properly tuning the value of the temperature, we have found that the 2-site system can almost perfectly mime,
as regards relevant properties such as the kinetic energy, the double occupancy, the energy, the specific heat,
the entropy and fundamental issues such as the metal insulator transition, the behavior of larger clusters and of
the infinite chain. The tuning of the temperature is necessary in order to get a comparable effective level spac-
ing (bigger the cluster, lower the spacing), i.e. to excite

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the correct levels: the relevant energy scales are present although the relative positions of the levels are affected by the size of the system (only two \( k \) points!). The very positive comparisons with exact results (Bethe ansatz, exact diagonalization) and numerical data (quantum Monte Carlo, Lanczos) support the idea that a lot of physics can be described and understood within this very small system, for which there is the possibility to know the analytic expressions for all the quantities under study. As regards the relevant scales of energy, this 2-site system has demonstrated to contain all the necessary ingredients to describe many features coming from the strong electronic correlations and also appearing in the lattice case. Two of the three relevant energy scales, which are thought to be present in the Hubbard model, naturally emerge: the local Coulomb interaction \( U \) and the spin-exchange one \( J = \frac{4t^2}{U} \); that is, in principle, extraneous to the original purely electrostatic Hamiltonian and is dynamically generated by the combined actions of the two terms of the Hamiltonian. As useful guide to better understand the low-energy dynamics we have also solved the \( t-J \) model and presented the solution in parallel with the one found for the Hubbard model.

This analysis, which has resulted to be really relevant by itself as we have got a much better understanding of some energy scales and internal parameter dynamics, has been worth to be performed also as a prelude of the lattice analysis. In fact, the eigenoperators we have found, both in the fermionic and the bosonic sectors, can be used in the lattice case as a basis for the Green’s functions. In the strongly correlated systems, the interactions can alter so radically the dynamics of the original particles that these latter lose completely their own identities [7]. Actually, some new objects are generated by the interactions and dictate the physical response. They are not so easy to be identified: their number, exact expression and relevance can only be suggested by the experience and, when available, by exact and/or numerical results. For instance, one can choose: the higher order fields emerging from the equations of motion, the eigenoperators of some relevant interacting terms, the eigenoperators of the problem reduced to a small cluster, etc. In the last years, we have been focusing our activity on the study of strongly correlated electronic models like Kondo, \( t-J \), \( p-d \), Hubbard by means of the Composite Operator Method [8–12] that is based on two main ideas: one is the use of composite fields as basis for our Green’s functions, in accordance to what has been discussed above, and the other one is the exploitation of algebra constraints (e.g., the Pauli principle, the particle-hole symmetry, the Ward-Takahashi identities, ...) to fix the correct representation of the Green’s functions and to recover the links among the spin and charge configurations dictated by the symmetries. It is worth noticing that the Composite Operator Method is exact in itself. An additional approximation treatment is needed when we deal with large or infinite degree-of-freedom systems; in this case we have to treat in an approximate way the otherwise intractable hierarchy of the equations of motion generated by the projection procedure. If no approximation is necessary (finite and reasonably small degree-of-freedom systems), the COM cannot do else than give the exact solution. According to this, the COM gives the exact solution also for the two systems under analysis in this manuscript: the two-site Hubbard and \( t-J \) models. Whenever, instead, we should resort to an approximate treatment to close the hierarchy of the equations of motion generated by the projection procedure, we expect some limitations connected with the chosen approximation. For instance, we get only the first moments correct if we truncate the equations of motion hierarchy [8]. On the other hand, it is really worth noting that we properly take into account: the interaction term of the Hamiltonian by using as basis operators its eigenoperators [13]; the short-range correlations by using as basic fields the eigenoperators of the problem reduced to a small cluster [14]; the presence of a Kondo-like singlet at low-energy by properly closing the equation of motion of an \( ad \) \( hoc \) chosen composite operator [15].

Obviously, we are aware that the exact diagonalization of this very small system takes less than one afternoon to any graduate student. Then, the reader could wonder why we decided to study such a system so in detail. Well, the reasons are many and some have been already pointed out above:

- Any graduate student can surely compute eigenstates and eigenvalues of these Hamiltonians in one afternoon, but the analytic computation of Green’s functions and correlation functions, in terms of the former eigenstuff, is not that straightforward as one can think. At the end of the day, the time saved in computing eigenstates and eigenvalues instead of eigenoperators is almost fully recovered if you also take into account the time needed by the computation of the physical properties (Green’s functions and correlations functions). Then, the possibility to have scalable information putting, altogether, almost the same effort become quite tempting for anyone. At any rate and for the sake of completeness, we report in Appendix A the expressions of Green’s functions and correlations functions in terms of eigenstates and eigenvalues.
- The knowledge of the exact eigenoperators of a system is invaluable as they could be used as correct starting point for the application of the projection methods [16–20] to strongly correlated systems whose minimal model [11] is the exactly solved one.
- The Green’s function formalism for composite operators is extremely complicated [11]. The 2-site Hubbard model can be used as toy model to fully explore this formalism and evidence the difficulties connected with the treatment of composite operators with non-canonical commutation relations. Within this system, the appearance of zero-frequency functions can be safely handled and resolved. The links among the different channels (fermion, charge, spin, pair) can be studied in detail.
- The 2-site Hubbard model, according to its status of minimal model [11], contains the main scales of energy related with the interactions present in the Hamiltonian. The exact solution in terms of eigenoperators