

Similarities between the t - J and Hubbard models in weakly correlated regimes

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Abstract. We present a comparative study of the Hubbard and $t - J$ models far away from half-filling. We show that, at such fillings the $t - J$ Hamiltonian can be seen as an effective model of the repulsive Hubbard Hamiltonian over the whole range of correlation strength. Indeed, the $|t/U| \in [0, +\infty[$ range of the Hubbard model can be mapped onto the finite range $|J/t| \in [2, 0]$ of the $t - J$ model, provided that the effective exchange parameter J is defined variationally as the local singlet-triplet excitation energy. In this picture the uncorrelated limit $U = 0$ is associated with the super-symmetric point $J = -2|t|$ and the infinitely correlated $U = +\infty$ limit with the usual $J = 0$ limit. A numerical comparison between the two models is presented using different macroscopic and microscopic properties such as energies, charge gaps and bond orders on a quarter-filled infinite chain. The usage of the $t - J$ Hamiltonian in low-filled systems can therefore be a good alternative to the Hubbard model in large time-consuming calculations.

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1 Introduction

In the last decade a renewed interest has been observed, in the study of simple models such as the Heisenberg model [1], Hubbard [2] or extended Hubbard model, the $t - J$ model [3], etc. This attraction is related to the synthesis by solid state chemists in the last two decades, of a large number of strongly correlated systems presenting very attractive low energy properties, often directly linked to the correlation effects. It is enough to say that these simple models are considered pertinent for the description of systems such as organic conductors [4] or high T_c super-conductors [3] to understand the importance of their study.

Among these models the Hubbard (or extended Hubbard) model is often considered as a reference since it has been built to reproduce the physics over the whole range of correlation strength, from delocalized to strongly correlated systems. The other models, for instance the spin models, are then considered as effective Hamiltonians of the Hubbard one under certain conditions. In particular the spin models, Heisenberg and $t - J$, are unanimously recognized as effective description of the valence physics in the large correlation limit ($U/t \rightarrow \infty$ where U is the on site Coulomb repulsion and t the nearest neighbor hopping integral). Indeed, in a half-filled,

one-band Hubbard model

$$H_{Hub} = t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

(where $a_{i,\sigma}^{\dagger}$, $a_{i,\sigma}$ and $n_{i,\sigma}$ are the usual creation, annihilation and number operators of an electron of spin σ on site i , and $\langle i, j \rangle$ symbolizes sites linked by the delocalization process), the probability of a site double occupancy rapidly decreases as $4t^2/U^2$, in the large U/t regime. The valence configurations involving sites double-occupancies are therefore negligible and can be excluded from an explicit representation, provided that their effects on the other configurations (involving only singly-occupied sites or vacant sites) is reproduced. As it is well known, this is exactly what is achieved by the Heisenberg Hamiltonian

$$\begin{aligned} H_{Heis} &= -J \sum_{\langle i,j \rangle} P (\mathbf{S}_i \cdot \mathbf{S}_j - 1/4 n_i n_j) P \\ &= -J \sum_{\langle i,j \rangle} P \left(\frac{a_{i,\uparrow}^{\dagger} a_{j,\downarrow}^{\dagger} - a_{i,\downarrow}^{\dagger} a_{j,\uparrow}^{\dagger}}{\sqrt{2}} \right) \\ &\quad \times \left(\frac{a_{i,\uparrow} a_{j,\downarrow} - a_{i,\downarrow} a_{j,\uparrow}}{\sqrt{2}} \right) P \\ &= -J \sum_{\langle i,j \rangle} P Sg^{\dagger}(i, j) Sg(i, j) P \end{aligned}$$

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where $Sg^\dagger(i, j)$ (resp. $Sg(i, j)$) is creating (annihilating) a singlet on the i, j bond and $P = \prod_i (\mathbb{1} - n_{i\uparrow}n_{i\downarrow})$ is the projector over all configurations excluding the double occupancy of a site.

Doping the system in holes (resp. in electrons) adds a new delocalization possibility for the particles which can thus be described by the so-called $t - J$ model

$$\begin{aligned} H_{t-J} &= t \sum_{\langle i,j \rangle} \sum_{\sigma} P \left(a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma} \right) P \\ &\quad - J \sum_{\langle i,j \rangle} P (\mathbf{S}_i \cdot \mathbf{S}_j - 1/4 n_i n_j) P \\ &= t \sum_{\langle i,j \rangle} \sum_{\sigma} P \left(a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma} \right) P \\ &\quad - J \sum_{\langle i,j \rangle} P \left(\frac{a_{i,\uparrow}^\dagger a_{j,\downarrow}^\dagger - a_{i,\downarrow}^\dagger a_{j,\uparrow}^\dagger}{\sqrt{2}} \right) \\ &\quad \times \left(\frac{a_{i,\uparrow} a_{j,\downarrow} - a_{i,\downarrow} a_{j,\uparrow}}{\sqrt{2}} \right) P. \end{aligned}$$

This simple derivation is very well known and the $t - J$ model is thus considered as the strongly correlated effective Hamiltonian of the Hubbard model away from half-filling.

In this paper we would like to come back on this assumption and show that the $t - J$ model can be seen as an effective model for the Hubbard Hamiltonian over the whole range of correlation strength, provided that one is far enough from half-filling.

The next section will be devoted to the physical justification and analytical development of the above assumption using the effective Hamiltonian theory [5]. Section three will assert the validity of the $t - J$ versus Hubbard equivalence for low-filling systems through numerical comparisons (energies, gaps, bond-orders) of a quarter-filled dimerized chain in the Hubbard and $t - J$ models, for the whole range of correlation and dimerization strengths. Eventually the last section will discuss the limitations of an effective Hamiltonian reduced to two-bodies interactions.

2 A variational effective exchange integral

We would like to start by drawing the attention of the reader on the reasons supporting the validity of the Heisenberg Hamiltonian as an effective model of the Hubbard Hamiltonian in the strongly correlated limit. The crucial point is that this is not the value of the correlation strength which is important, but rather the fact that the probability of sites double-occupancies is very small in the ground state and low lying excited states wave functions. The relevance of this distinction appears mainly away from half-filling. Indeed, while in half-filled systems the low probability of the double occupancy is a direct consequence of the large correlation, far from half-filling this is no longer the case. Actually, for low-filled systems (and

equivalently by hole particle symmetry for nearly-filled systems) the configurations associated with site(s) double-occupancies are negligible independently of the correlation strength. One can indeed verify that even in the non interacting regime ($U = 0$), where the double occupancies on a site are the most probable over the whole range of correlation strength, the wave-function of a η -filled system yields a statistical weight for double occupancies on a site of η^2 . Although it does correspond to a quite-large contribution at half-filling ($\eta^2 = 1/4$), it becomes rapidly very small when the filling is reduced, with a value of only $\eta^2 = 1/16 = 0.0625$ for the quarter-filling case. Since the electron-electron correlation can only reduce this number, it seems justified to exclude the explicit reference to double-occupancies in the wave-function of low-filled (or nearly-filled, using the hole/particle symmetry) systems. However, as in the Heisenberg limit, simply projecting out the double occupancies on a site would not give the correct physics and the effects of these double occupancies on the other states should be effectively reproduced. As we have seen, this is exactly the role of the effective exchange integral in the Heisenberg model as well as the $t - J$ model, that is to lower the local singlet states compared to the local triplet ones, setting the energy of the neutral representation of a local singlet $(|a\bar{b}\rangle - |\bar{a}b\rangle)/\sqrt{2}$ to $-J$ compared to the local triplet $(|a\bar{b}\rangle + |\bar{a}b\rangle)/\sqrt{2}$ that lies at 0. In the strongly correlated limit the singlet-triplet excitation energy is evaluated perturbatively. However, since we would like to derive an effective model valid over the whole range of correlation strength, perturbative evaluations of the effective exchange have to be excluded. We will therefore use locally the principle of the effective Hamiltonian theory [5] (reproduction by the effective Hamiltonian of the exact eigen-energies and projection of the exact eigenstates over the model space: $H_{\text{eff}} P \Psi_{\text{exact}} = E_{\text{exact}} P \Psi_{\text{exact}}$) in order to derive a variational evaluation of the main effects of double-occupancies on a site (from now on denoted as DOC) on the low energy states (for a more detailed description one can refer to Ref. [6]).

Summarizing the previous discussion we can conclude that far away from half-filling, the configurations including site(s) double-occupancies can be excluded from an explicit treatment, provided that their main effect, the lowering of the local singlets compared to the local triplets, are reproduced by an effective exchange integral. We therefore see that the Hubbard Hamiltonian can be modeled by the $t - J$ Hamiltonian in the low-filling regime, providing a non perturbative effective exchange integral, $J(t, U)$. The simplest way to derive $J(t, U)$ is to impose that it reproduces the variational local singlet-triplet energy difference on a bond (two sites, two electrons). The Hubbard model yields $E(Sg) = (U - \sqrt{U^2 + 16t^2})/2$, $E(Tp) = 0$, it comes

$$J(t, U) = \frac{U - \sqrt{U^2 + 16t^2}}{2}. \quad (1)$$

Let us note that we retrieve for large values of t/U the perturbative evaluation of J : $-4t^2/U$ as the first term of the Taylor expansion in t/U . For the non-correlated limit

the expansion should be done in terms of U/t and it yields

$$J = \frac{U - \sqrt{U^2 + 16t^2}}{2} \simeq -2|t|$$

that is the value of J for the super-symmetric point. The super-symmetric point of the $t - J$ model (the only one to be exactly soluble [7]) therefore appears as an effective description — on the model space projecting out all site(s) double-occupancies — for the tight-binding Hamiltonian. In this perspective the results of Yokoyama *et al.* [8] about the super-symmetric point properties showing that it realizes a Fermi-Liquid state or free Luttinger liquid and behaves in all points as a free-electrons gas seem quite natural. Meanwhile, the effective Hamiltonian theory states that the ground-state wave-function of a properly defined effective Hamiltonian should be the projection over the model space of the exact Hamiltonian one [5]. This property agrees nicely with the results of Yokoyama *et al.* [9] that shows that the Gutzwiller state is the ground state of the $t - J$ model at the super-symmetric point. In other words the projection of the free-electron wave-function onto the space excluding all double occupations on a site is the $t - J$ ground state for $J(t, U = 0)$.

We would like to point out that the effective exchange $J(t, U)$ valid to represent the repulsive Hubbard model is bounded and varies from $J(t, U = 0) = -2|t|$ for the non correlated limit to $J(t, U = \infty) = 0$ for the strongly correlated limit. Let us note that these boundaries excludes the whole range of parameters for which phase separation phenomena occur. It should also be noted that the arguments leading to the effective exchange $J(t, U)$ is not specific to the dimension one and should be expected to hold in all dimensions, at least for non frustrated systems.

Apart from the effective exchange effect, it is known from perturbative expansion at large correlation strength, that the DOC induce effective 3 bodies interactions of lesser importance. This point will be discussed in section four and a way to obtain a variational evaluation of these terms will be proposed.

3 The dimerized quarter-filled chain

In this section we will show numerically that the equivalence between the Hubbard and $t - J$ models really holds for all values of the correlation strength and for all possible dimerizations. For this purpose we will compare the following low energy properties of a quarter-filled chain in the two models.

- The behavior of the total energy per site as a function of t/U and the dimerization amplitude δ . This point can be crucial for a good representation of phase transitions in systems presenting a more complex topological graph.
- The charge gap. This criterion will attest for a good low energy spectroscopic behavior.
- The effective bond order, as it testifies for the wave function behavior.

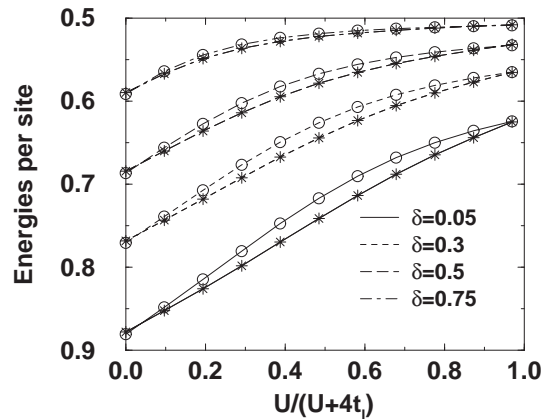


Fig. 1. Energies per site as a function of $U/(U + 4|t_l|)$ and δ for the Hubbard (stars) and $t - J$ (circle) models, in t_l units.

The calculations will be done using the infinite systems Density Matrix Renormalization Group (DMRG) method [10]. We choose the number of states kept in the renormalized blocks in such a way that for each model the 10-sites system is treated exactly. The Hubbard model will therefore be described with 256 states and the $t - J$ one with only 100 states. These numbers of states kept per renormalized block correspond to a sum of the discarded states weights always smaller than 1×10^{-7} , for the Hubbard model, and smaller than 1×10^{-5} , for the $t - J$ model. These results are for small dimerization values and small correlation values, that is for the most difficult cases in terms of the DMRG algorithm convergence and precision. These small values of the discarded states weight insures the good convergence of our results, even-though we did use the infinite size DMRG algorithm.

The dimerization amplitude is defined as

$$\delta = (t_l - t_w) / t_l$$

where t_l is the large hopping integral and t_w is the weak one.

3.1 Energies per site

The energies per site have been extrapolated with respect to the number of sites in the chain and are presented in Figure 1 as a function of the correlation strength $U/(U + 4|t_l|)$. Different values of the dimerization factor δ have been investigated starting from the weakly dimerized chain $\delta = 0.05$ up to the strongly dimerized one $\delta = 0.75$.

We see in Figure 1 that the agreement between the two models is quite good. Both the variations as a function of the correlation strength and the dimerization amplitude are well reproduced. The maximal relative error between the Hubbard and $t - J$ total energies per site is only 0.03. As expected, the large $U/|t_l|$ asymptotic limit is well reproduced by the $t - J$ model for all values of the dimerization. A little less obvious is the very good numerical accuracy found for the non-interacting limit. The relative error

found between our computed $t-J$ values and the *exact* free electron solution is bounded by 0.004 and can probably be imputed for its greatest part to the DMRG procedure (which is known to have its worse convergence properties for the non correlated limit). Actually, the largest errors occur in the region of intermediate correlation strength ($U/t \simeq 4$) and for small dimerization. As the dimerization increases and for a given U/t ratio, the $t-J$ model fits better and better the Hubbard one. This point can be easily understood if one remembers that the three bodies terms, neglected in the $t-J$ Hamiltonian, should decrease as a function of the dimerization amplitude.

3.2 Charge gaps

We computed the charge gaps Δ_ρ , as the extrapolated difference toward the infinite system limit, between the ionization potential (IP) and the electron affinity (EA). If $E(N_{site}, N_e)$ is the energy of a finite N_{site} sites system with N_e electrons, the charge gap is written as the following:

$$\Delta_\rho = \lim_{N_{site} \rightarrow \infty} \{E(N_{site}; N_{site}/2 + 1) + E(N_{site}; N_{site}/2 - 1) - 2E(N_{site}; N_{site}/2)\}.$$

The Hubbard and $t-J$ gaps are presented in Figure 2 as a function of the correlation strength $U/(U+4|t|)$, and for 4 different values of δ .

One sees immediately that the dimerization gaps exhibit the same general behavior for the Hubbard and the $t-J$ model. The response both as a function of the dimerization amplitude and the correlation strength are very similar and quite close in absolute values even if the gaps are slightly larger in the $t-J$ model than in the Hubbard one. For the large U asymptote in the Hubbard model, it is noticeable that the DMRG procedure fails to give good estimations of the dimerization gaps. This failure has already been observed [11] and may find its origin in a lack of numerical accuracy when the absolute values involved in the gap calculations become too large. For large- U and large- δ , Penc and co-workers [12] have shown that the charge gaps are expected to coincide with a $2 \times \delta$ asymptote. It can be seen from Figure 2 that this large- U limit is rather well verified even for intermediate δ . It is noticeable that in the non-interacting limit the $t-J$ effective model exhibits the proper exponential behavior as a function of the correlation strength and the dimerization amplitude.

3.3 Bond orders

We computed the bond orders for the Hubbard model and $t-J$ model. However one can expect that the elimination of the explicit reference to the DOC in the wavefunction will strongly affect the values of the bond order. Indeed, over a $\langle i, j \rangle$ bond, the different configurations that contribute to the bond order are

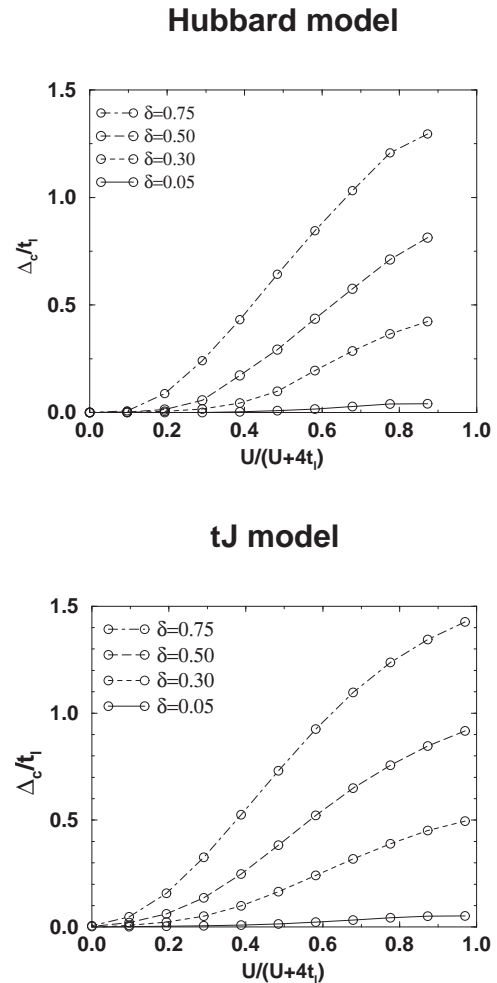


Fig. 2. Charge gaps Δ_ρ in t_l units calculated within the Hubbard and $t-J$ models. Each curve corresponds to a different value of δ , going from the weakly dimerized limit $\delta = 0.05$ to the strongly dimerized one $\delta = 0.75$

- the local one-electron doublets which are explicitly treated in the $t-J$ model, and contribute for $1/2$ for the bonding one and $-1/2$ for the anti-bonding one,
- the local triplet which is explicitly treated in the $t-J$ model and has a zero contribution to the bond-order,
- the essentially neutral, ground state singlet which is *effectively* treated in the $t-J$ model and has a zero contribution to the bond-order when the DOC states are ignored, but has a real contribution of $\frac{4|t|}{\sqrt{U^2+16t^2}} = \frac{2|tJ|}{t^2+J^2}$ when the DOC are taken into account,
- the essentially ionic singlets that are ignored in the $t-J$ model since their contribution is very small in the wave function and has a real contribution to the bond order of $\frac{-4|t|}{\sqrt{U^2+16t^2}} = \frac{-2|tJ|}{t^2+J^2}$ for the symmetric one and of 0 for the antisymmetric one,
- the three electrons doublets that are ignored in the $t-J$ model because of their very low occurrence in the system wave function and should have a contribution to the bond order of $1/2$ for the bonding one and of $-1/2$ for the anti-bonding one.

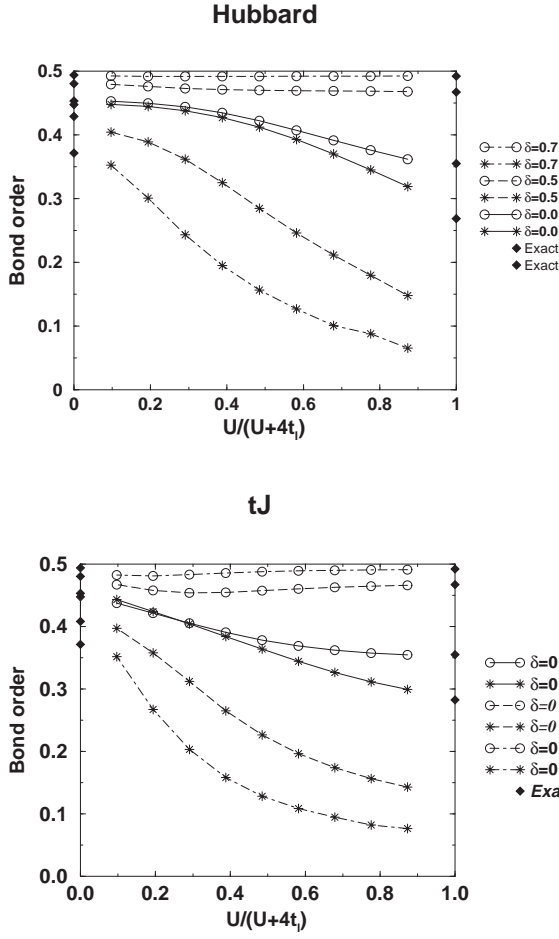


Fig. 3. Bond orders p calculated within the Hubbard model and renormalized bond order calculated within the t - J model. Circles correspond to the short bonds (SB) and stars to the long bonds (LB).

One sees immediately that in order to have a reasonable evaluation of the bond order in the t - J model one should at least add an effective term setting up to the correct value the contributions of the quite probable local neutral singlets. We will therefore define the effective t - J bond order as the true t - J bond order plus the exact contribution of the essentially neutral singlets, that is

$$\hat{p} = \frac{1}{2} \sum_{\langle i,j \rangle} \sum_{\sigma} \left(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma} \right) + \frac{2|tJ|}{t^2 + J^2} \sum_{\langle i,j \rangle} Sg^{\dagger}(i,j) Sg(i,j).$$

Figure 3 shows the bond-order for the Hubbard model and the effective bond-order for the t - J model, for the whole range of correlation strength and dimerization values.

The effective bond order of the t - J model behaves reasonably well both as a function of the correlation strength and the dimerization. Both the strongly correlated limit and the $U = 0$ limit of the Hubbard model are very well

reproduced by the t - J model. As for the energies, the major discrepancies between the two models are in the moderately delocalized regime, typically between $U/t = 2$ and $U/t = 4$, and for low dimerizations where the effective t - J bond order is slightly too rapidly decreasing.

One can conclude from the previous results that the t - J model reproduces quite well the low energy physics of the Hubbard model in the low filling regime, over the *whole range* of the correlation strength, provided that the exchange integral as well as the other observables are defined so that to effectively take into account the main effects of the DOC states.

4 The three bodies terms

From the perturbative expansion of the Hubbard model in the strong correlation limit, we know that the exact effective model excluding all DOC states should involve three, four, \dots , n bodies terms. After the dominant first neighbor effective exchange of the t - J model, second neighbor hopping and three bodies terms appear at the second order of perturbation. These secondary terms which are negligible near the complete or the very low fillings have a maximal probability of occurrence at $1/3$ filling (at $U = 0$). However their relative importance compared to the local singlet or triplet terms raises as $(1-\eta)^2$ as a function of the filling η . In the very low filling regime, these terms are therefore negligible, however in the same way as the local singlets and triplets. In the low, but not too low filling regime, one can expect that these terms may account for some secondary corrections. Indeed, in the $1/4$ -filling regime used to exemplify this work, they have (for $U = 0$) a total probability of occurrence of 0.0198. One can therefore expect that these terms may account for a large amount of the small quantitative discrepancies observed between the Hubbard and effective t - J models. Therefore, if one would like a more quantitative representation of the Hubbard model on the states excluding all double occupancies on a site, one should add to the t - J Hamiltonian a second neighbor hopping and a three body term.

$$\begin{aligned} H_{3b} = & t \sum_{\langle i,j \rangle} \sum_{\sigma} P \left(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma} \right) P \\ & - J/2 \sum_{\langle i,j \rangle} P \left(a_{i,\uparrow}^{\dagger} a_{j,\downarrow}^{\dagger} - a_{i,\downarrow}^{\dagger} a_{j,\uparrow}^{\dagger} \right) \left(a_{i,\uparrow} a_{j,\downarrow} - a_{i,\downarrow} a_{j,\uparrow} \right) P \\ & + t_2 \sum_{\langle i,j,k \rangle} \sum_{\sigma} P \left(a_{i,\sigma}^{\dagger} a_{k,\sigma} + a_{k,\sigma}^{\dagger} a_{i,\sigma} \right) n_{j,\bar{\sigma}} (1 - n_{j,\sigma}) P \\ & + K \sum_{\langle i,j,k \rangle} P \left(a_{i,\sigma}^{\dagger} a_{k,\bar{\sigma}} + a_{k,\sigma}^{\dagger} a_{i,\bar{\sigma}} \right) a_{j,\bar{\sigma}}^{\dagger} a_{j,\sigma} (1 - n_{j,\bar{\sigma}}) P \end{aligned}$$

where the sum over $\langle ijk \rangle$ runs over all three nearest neighbor sites. As for the effective exchange $J(t, U)$ of the t - J Hamiltonian, the J , t_2 and K parameters of H_{3b}

can be variationally derived as a function of Hubbard t and U , from the low energy spectroscopy (between the six essentially neutral states) of the three sites, two electrons fragment. It comes

$$J = \frac{U}{2} - \frac{\sqrt{U^2 + 16t^2} + \sqrt{U^2 + 8t^2}}{4}$$

$$t_2 = -K = \frac{\sqrt{U^2 + 16t^2} - \sqrt{U^2 + 8t^2}}{8}.$$

It should be noted that we are no more in a $t - J$ model and that the free electrons system now maps onto a three body model with parameters $J = (1 + \sqrt{2})|t|$, $t_2 = (1 - \sqrt{2})/2|t|$ and $K = -(1 - \sqrt{2})/2|t|$.

5 Conclusion

The $t - J$ model is a well known effective Hamiltonian of the Hubbard model in the strongly correlated limit. We have shown in this paper that the $t - J$ model can be seen as such, as long as the double occupancies of a site have a very low probability of occurrence in the ground and low excited states of the system. This is in particular the case for low filled bands (or nearly filled band using electron-hole symmetry), whatever the value of the correlation strength. We have proposed a variational evaluation of the effective exchange $J(t, U)$ so that it insures the proper excitation energy between the local singlets and triplets. Using this effective $t - J(t, U)$ model, we have shown on an infinite quarter filled chain, that the total energy per site, the charge gaps as well as the bond-orders behave similarly than in the Hubbard model, over the whole range of correlation strength and dimerization. The agreement is not only qualitative, but also quantitative, the small discrepancies seen in the intermediate low (but not too low) correlation regime being analyzed as due to the neglected three bodies terms. It is interesting to point out that the super-symmetric point of the $t - J$

model corresponds to the effective representation of the uncorrelated limit, $U = 0$, yielding as a natural consequence to the effective Hamiltonian theory, its surprising Fermi liquid behavior.

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