# Dynamical Symmetry Enlargement versus Spin-Charge Decoupling in the One-Dimensional SU(4) Hubbard Model

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We investigate dynamical symmetry enlargement in the half-filled SU(4) Hubbard chain using nonperturbative renormalization-group and quantum Monte Carlo techniques. A spectral gap is shown to open for arbitrary Coulombic repulsion $U$. At weak coupling, $U \lesssim 3t$, a SO(8) symmetry between charge and spin-orbital excitations is found to be dynamically enlarged at low energy whereas at strong coupling, $U \gtrsim 6t$, the charge degrees of freedom dynamically decouple. The crossover between these regimes is discussed.

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In strongly correlated electronic systems, the presence of additional dynamical degrees of freedom out of the usual spin and charge ones is expected to play an important role in a number of complex systems. This is the case, for example, of some $d$-electron systems [1], $C_{60}$-based materials [2] and also various ladder-type compounds [3], for which low-energy excitations cannot be constructed from a single effective orbital per site (one band). An important question that arises is to know whether or not there exist *generic* features associated with multi-orbital effects. Such a question is nontrivial since it is known that the lack of symmetry in multi-orbital problems [beyond the usual SU(2) spin invariance] is responsible for the presence of many independent couplings and, therefore, a wide range of problem-dependent physical behaviors could be expected. However, at sufficiently low energy, it may happen that the effective symmetry is increased, thus considerably simplifying the description of the problem. This is of course what happens in a critical (gapless) model. In the more general case where a spectral gap is present, the possibility of such a dynamical symmetry enlargement (DSE) at low energy is clearly nontrivial. Recently, Lin, Balents, and Fisher [4] have emphasized that DSE is likely to be a generic tendency of the perturbative (one-loop) renormalization-group (RG) flow in their study of the half-filled two-leg Hubbard ladder. However, since in a gapped system DSE is a *strong* coupling effect, one may thus question the reliability of perturbation theory [5]. Clearly, in view of the importance that such a DSE phenomenon might have in our understanding of complex systems, a nonperturbative investigation is called for, and it is the purpose of this Letter to present such a study.

In the following, we investigate the DSE phenomenon using nonperturbative RG and quantum Monte Carlo (QMC) simulations for the simplest one-dimensional half-filled two-band Hubbard model, where spin and orbital degrees of freedom play a *symmetrical* role. The corresponding SU(4) Hubbard model reads as follows:

$$\mathcal{H} = -t\sum_{i,a\sigma}(c^{\dagger}_{i,a\sigma}c_{i+1,a\sigma} + \mathrm{H.c.}) + \frac{U}{2}\sum_{i}\left(\sum_{a\sigma}n_{i,a\sigma}\right)^2, \tag{1}$$

where $c^{\dagger}_{i,a\sigma}$ creates an electron with spin $\sigma = (\uparrow, \downarrow)$ and orbital index $a = (1, 2)$ at the $i$th site, and $n_{i,a\sigma} = c^{\dagger}_{i,a\sigma}c_{i,a\sigma}$. The total symmetry group of (1) is $\mathrm{U}(4) = \mathrm{U}(1)_{\mathrm{charge}} \otimes \mathrm{SU}(4)_{\mathrm{spin\ orbital}}$; it is the maximal symmetry allowed for a two-band Hubbard model. A simple one-loop perturbative analysis [4] would predict that, at half-filling, a SO(8) symmetry between *charge* and spin-orbital degrees of freedom is likely to be dynamically enlarged at low energy. Such a DSE pattern, $\mathrm{U}(4) \to \mathrm{SO}(8)$, is highly nontrivial since one naturally expects the charge degrees of freedom to decouple at sufficiently large $U$. Indeed, in the limit $U \gg t$, the Hamiltonian (1) reduces, at half-filling, to an antiferromagetic (AFM) Heisenberg model [where the spin operators act on the six-dimensional antisymmetric representation of SU(4)]. It is precisely the interplay between the small-$U$ predicted SO(8) regime and the large-$U$ charge-decoupled Heisenberg limit which is considered here.

The low-energy effective field theory is obtained, as usual by performing the continuum limit. The $\mathrm{U}(1)_{\mathrm{charge}}$ charge sector is described, in a standard way, by a single bosonic field $\Phi_c$ and its dual field $\Theta_c$. There are many equivalent ways to describe the spin-orbital excitations in the $\mathrm{SU}(4)_{\mathrm{spin\ orbital}}$ sector, and it is most convenient to represent them by six real (Majorana) fermions $\xi^a$, where $a = (1, \ldots, 6)$ [6]. We find for the low-energy effective Hamiltonian

  

$$\mathcal{H} = \frac{v_c}{2}\left[\frac{1}{K_c}(\partial_x\Phi_c)^2 + K_c(\partial_x\Theta_c)^2\right] - \frac{iv_s}{2}\sum_{a=1}^{6}(\xi_R^a\partial_x\xi_R^a - \xi_L^a\partial_x\xi_L^a) + \pi g_s\left(\sum_{a=1}^{6}\kappa^a\right)^2 - 2ig_{sc}\cos(\sqrt{4\pi}\Phi_c)\sum_{a=1}^{6}\kappa^a, \quad (2)$$

where $\kappa^a = \xi_R^a\xi_L^a$, $g_s = -g_{sc} = -U/2\pi$, and $v_s = v_F + g_s$, $v_F = 2t$ being the Fermi velocity. In Eq. (2), the Luttinger exponent $K_c = 1/\sqrt{1 + 2g_c/v_F}$ and the charge velocity $v_c = v_F\sqrt{1 + 2g_c/v_F}$ depend on the charge coupling $g_c = 3U/2\pi$. The low-energy effective field theory (2) describes the interaction between a SO(6) Gross-Neveu (GN) model, associated with spin-orbital degrees of freedom, and a Luttinger liquid Hamiltonian in the charge sector. The interaction term, with coupling constant $g_{sc}$, is an umklapp contribution that comes from the $4k_F$ part of the Hamiltonian density and is present only at half-filling $k_F = \pi/2$. In sharp contrast with the half-filled SU(2) Hubbard model and the SU(4) case at quarter-filling [7], there is *no* spin-charge separation at low energy for half-filling. Spin orbital and charge degrees of freedom remain strongly coupled through the $4k_F$ umklapp process. At this point it is worth stressing that there exists a higher-order umklapp term ($8k_F$ process) $\mathcal{V}_c = y\cos(\sqrt{16\pi}\Phi_c)$, which depends only on the charge degrees of freedom. Although this operator, with scaling dimension $\Delta = 4K_c$, is strongly irrelevant at small $U$, it may become relevant at sufficiently large $U$. As we shall see, this contribution is at the heart of the physics of the SU(4) Hubbard model in the large $U$ limit.

A simple one-loop RG calculation reveals that the couplings $g_a = (g_c, g_s, g_{sc})$ flow at strong coupling. In particular, as $g_c$ blows up at low energy, $K_c$ inevitably decreases until $\mathcal{V}_c$ becomes relevant. Thus, the nature of the low-energy physics depends on the balance between the two umklapp operators with very different properties. Clearly, nonperturbative methods are called for. In this respect, Gerganov *et al.* [8] have provided a RG framework which allows one to compute the RG $\beta$ function *to all order* in perturbation theory for a large class of one-dimensional models with current-current interactions. We have applied their formalism to the Hamiltonian (2) and obtained the resummed $\beta$ function [9]. Neglecting velocity anisotropy, we get

$$\dot{g}_c = 24(g_c - 2)^2\frac{g_{sc}^2}{(g_{sc}^2 - 4)^2},$$
$$\dot{g}_s = \frac{16g_s^2}{(g_s + 2)^2} + 8(g_s - 2)^2\frac{g_{sc}^2}{(g_{sc}^2 - 4)^2}, \quad (3)$$
$$\dot{g}_{sc} = \frac{4g_{sc}}{4 - g_{sc}^2}\left[12 - (g_{sc}^2 + 4)\left(\frac{1}{g_c + 2} + \frac{5}{g_s + 2}\right)\right],$$

where $\dot{g}_a = \partial g_a/\partial t$, $t$ being the RG "time," and $g_a \to g_a/v_F$. In the absence of the umklapp contribution $\mathcal{V}_c$, we find that the RG flow crucially depends on $g_c$ as follows. In the weak-coupling regime, at small enough $U/t$ such that $g_c \leq 2$, all the couplings converge to the *same* value, $g_a(t^*) = 2$, at some finite RG time $t^*$. On the other hand, when $g_c > 2$, one enters a regime where perturbation theory is meaningless.

*Weak-coupling regime.*—When $g_c < 2$, much can be said on the low-energy physical properties of the model (1). Indeed, integrating the flow up to $t^*$, one finds that the Hamiltonian (2) at that scale reduces to the SO(8) GN model:

$$\mathcal{H}^* = -\frac{iv}{2}\sum_{a=1}^{8}(\xi_R^a\partial_x\xi_R^a - \xi_L^a\partial_x\xi_L^a) + 2\pi v\left(\sum_{a=1}^{8}\kappa^a\right)^2, \quad (4)$$

where we have refermionized the charge degrees of freedom in terms of two real fermions $\xi^{7,8}$: $(\xi^7 + i\xi^8)_{R(L)} \sim \exp(\pm i\sqrt{4\pi}\Phi_{cR(L)})$. The equivalence at low energy between (1) and (4) is a manifestation of the DSE $U(1)_{\rm charge} \otimes SU(4)_{\rm spin\ orbital} \to SO(8)$. This SO(8) enlarged symmetry, which has been first predicted using a 1-loop RG calculation in [4], is shown here to hold beyond perturbation theory provided $g_c < 2$. For higher values of $g_c$, the higher-umklapp term $\mathcal{V}_c$ plays a prominent role at low energy and, as we shall see, is responsible of the dynamical decoupling of the charge degree of freedom. One of the main interests of the emergence of this SO(8) symmetry stems from the fact that the model (4) is integrable and a large amount of information can be extracted from the exact solution [4,10]. The low-lying spectrum of the SO(8) GN model (4) is fully gapped and consists of three distinct octets with the same mass $m \sim te^{-t/U}$. The fundamental fermion octet, associated with the Majorana fermions $\xi^a$ of Eq. (4), is made of two charged $\pm 2e$ spin-orbital singlets, called cooperons, and six spin-orbital excitations which transform according to the self-conjugate representation of SU(4) with dimension 6. The remaining two octets are of kinks type. In particular, the excitations of the SU(4) Hubbard model (1), carrying the quantum numbers of the lattice fermions $c_{i,a\sigma}$, are represented by eight of these kinks. In addition, there are 28 bosonic states organized as a rank-2 SO(8) antisymmetric tensor and a singlet, all of mass $\sqrt{3}m$, which can be viewed as bound states of the fundamental fermions or of the kinks states. The massive phase corresponding to the SO(8) GN model (4) is a spin-Peierls (SP) phase as it can be readily shown by considering the order parameter $\mathcal{O}_{\rm SP} = \sum_{i,a\alpha}(-1)^i c_{i,a\alpha}^\dagger c_{i+1,a\alpha}$, which has a nonzero expectation value $\langle\mathcal{O}_{\rm SP}\rangle \neq 0$. The ground state of (4) is thus doubly degenerate and spontaneously breaks the lattice translation symmetry. The striking feature is that, despite of this dimerization, both electronic and spin-orbital excitations are *coherent*; i.e., they contribute to sharp peaks in various spectral functions. This result stems from the existence in the exact spectrum of (4) of states that have the same quantum numbers as the electron and spin-orbital operators $c^\dagger_{i,a\sigma}c_{i,b\beta}$. In particular, the dynamical structure spin factor of the system displays a sharp peak at energy $\omega = \sqrt{3}m$, corresponding to an excitation of one of the bosonic states of the SO(8) theory. In this respect, the half-filled SU(4) Hubbard model is predicted to be a fully coherent gapped dimerized liquid at weak coupling.

Although the RG Eq. (3) is nonperturbative in nature, it remains to investigate the effect of neglected symmetry-breaking operators such as the higher-umklapp term $\mathcal{V}_c$ and chiral interactions that account for velocities anisotropy. For small symmetry-breaking terms, the SO(8) multiplets will be adiabatically deformed and split into $U(1)_{\rm charge} \times SU(4)_{\rm spin\ orbital}$ multiplets; the SO(8) symmetry is only realized approximately at weak enough couplings. At small $U/t$ the splittings are exponentially small, but we expect perturbation theory to break down as $U$ increases, even when $g_c < 2$. The reason stems from the neglected umklapp operator $\mathcal{V}_c$, which becomes relevant before one reaches the SO(8) symmetry restoration point as $\Delta < 2$ when $g_c > 3/2$. We thus expect the SO(8) regime to hold approximately up to some critical value $U_c$, from which a very naive estimate can be obtained using the bare value of $g_c$: $U_c \sim 2\pi t$.

In order to check our theoretical predictions, we have performed extensive $T = 0$ QMC simulations of the SU(4) Hubbard model (1) at half-filling for a wide range of $U/t$. Following the work done in Ref. [7] in the quarter-filled case, we have computed all gaps associated with the SO(8) tower of states. We discuss here our results for three of them: $\Delta_1$, which is the gap to the one-particle excitation $c^\dagger_{i,a\sigma}$, $\Delta_s$, which is the spin-orbital gap associated with the excitations $c^\dagger_{i,a\sigma}c_{i,b\mu}$, and, finally, the cooperon gap $\Delta_c$, which is the gap to a spin-orbital singlet state of charge $2e$. The latter excitation is a striking feature of the SO(8) spectrum and is not simply related to electronic excitations on the lattice. For example, the cooperon comes into pairs from the charge $4e$ excitation $\Pi_{a\sigma}c^\dagger_{i,a\sigma}$. We have computed the cooperon gap $\Delta_c$ as half the gap of this state. The exact spectrum of (4) imposes the highly nontrivial predictions for the ratios $(\Delta_1/\Delta_c)_{SO(8)} = 1$ and $(\Delta_s/\Delta_c)_{SO(8)} = \sqrt{3}$ (note that the spin-orbital excitations we are considering are *bound states* of two one-particle excitations). Strong deviations from these theoretical predictions will be a signature of the failure of the increased SO(8) symmetry. We show in Fig. 1 our results for $\Delta_1(U)$, $\Delta_s(U)$, and $\Delta_c(U)$, for values of $U/t$ ranging from 0.5 to 20. The extrapolation to the thermodynamical limit has been performed using lattice sizes $L = 8, 16, 32, 48, 64$, and the errors on the gaps range from $10^{-2}$ at small $U/t$ to $10^{-3}$ at large $U/t$. Two asymptotic regimes are identified: a small $U/t$ regime and a large $U/t$ regime, where spin orbital and charge degrees of freedom clearly separate. Both regimes are most easily seen on the spin gap $\Delta_s(U)$, behavior (inset of Fig. 1) which increases until it reaches a maximum around $U/t \sim 6$ and then decreases smoothly to zero as $U/t \to \infty$. Clearly the SO(8) regime is expected to show off at small $U/t$. In Fig. 2 we plot the ratio $(\Delta_1/\Delta_c)(U/t)$. One observes a clear saturation of the ratio at the SO(8) value as $U$ decreases below $U \sim 3.5t$. Other gap ratios, not presented here [9], show also a SO(8) saturation in the regime $U \lesssim 3.5t$. These results strongly support the existence of a SO(8) DSE in a regime where the gaps are not infinitesimally small ($\Delta_s \sim 0.1t$–$0.2t$). Above $U \sim 3.5t$, the ratio shows a departure from its SO(8) value. Though such a behavior may be attributed to level splitting due to symmetry-breaking operators at small $U/t$, this is certainly not the case above $U \sim 6t$, where $\Delta_1/\Delta_c$ saturates at the value 1/2. It is difficult from our results to give a precise value to $U_c$ above which the SO(8) regime is lost, but we can give an estimate $3t \leq U_c \leq 6t$. Notice that the upper value is in agreement with our rough estimate of $U_c = 2\pi t$ based on a scaling argument.

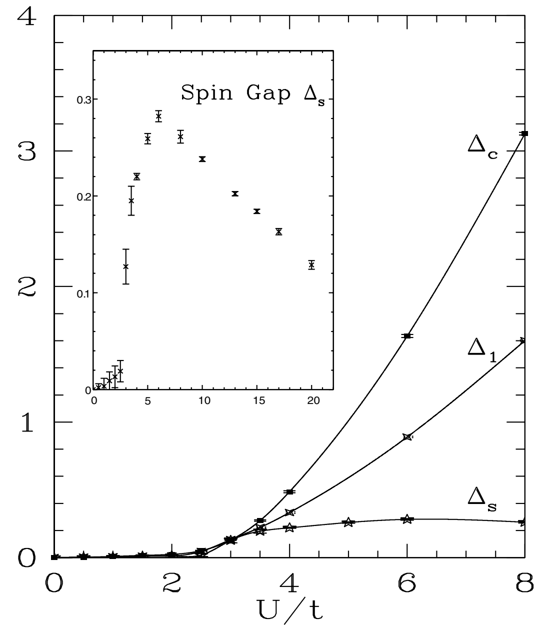


FIG. 1. One-particle gap $\Delta_1$, spin-orbital gap $\Delta_s$, and cooperon gap $\Delta_c$ as a function of $U/t$; inset: $\Delta_s$ gap as function of $U/t$.

*Strong-coupling regime.*—When $U/t \gg 1$, there is a clear separation between spin orbital and charge degrees since $\Delta_c \gg \Delta_s$ (see Fig. 1). The umklapp term $\mathcal{V}_c$, which depends only on the charge degrees of freedom, now becomes much more relevant than the $4k_F$ coupling, and charge fluctuations are strongly suppressed by this process. Integrating out the charge degrees of freedom, the low-energy effective Hamiltonian in the spin-orbital sector reduces to a massive SO(6) GN model:

$$\mathcal{H}_{\rm SO} \simeq -\frac{iv_s}{2}\sum_{a=1}^{6}(\xi^a_R\partial_x\xi^a_R - \xi^a_L\partial_x\xi^a_L) - iM\sum_{a=1}^{6}\kappa^a + G_s(U)\left(\sum_{a=1}^{6}\kappa^a\right)^2, \quad (5)$$

where $M > 0$ and $G_s(U)$ is a negative effective coupling

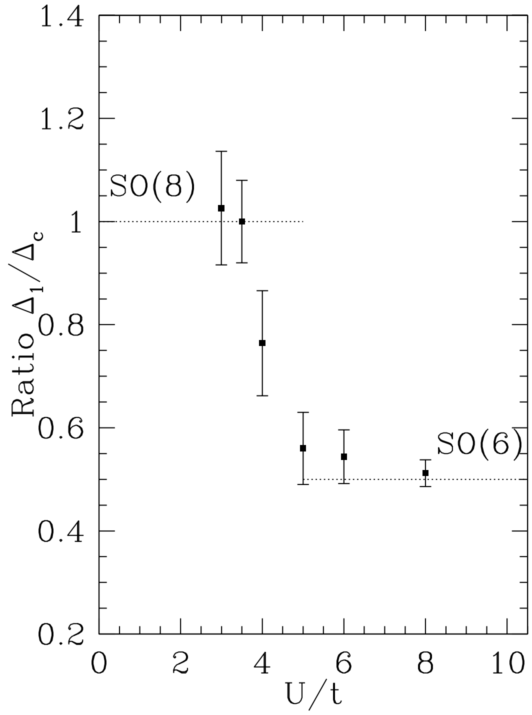


FIG. 2. Gap ratio $\Delta_1/\Delta_c$ as a function of $U/t$.

at large $U/t$. The Hamiltonian (5) describes *six* massive Majorana fermions with a weak repulsion. One can show, using Eq. (5), that $\langle \mathcal{O}_{\rm SP} \rangle \neq 0$ so that the ground state is still in a SP phase. Neglecting charge fluctuations, this dimerized phase, with broken translational symmetry, can be simply understood as a set of nearest-neighbor SU(4) $\sim$ SO(6) spin-orbital singlet bonds. There is thus a continuity between weak and strong coupling with respect to the nature of the ground state. However, there is a striking difference between the SO(8) regime and this strong-coupling phase, called SO(6) regime, at the level of the coherence of excitations. The excitation spectrum of the model (5) for $G_s < 0$ consists of massive fermions $\xi^a$, which are the SU(4) dimerization kinks, and their multiparticle excitations. In particular, there are no bound states so that the spin-orbital dynamical structure factor exhibits a two-particle continuum; the spin-orbital excitations are now *incoherent*. Apart from these neutral excitations, there are massive modes corresponding to solitons in $\Phi_c$ with charge $q = \pm e$ coupled with zero modes of the Majorana fermions $\xi^a$ of Eq. (5). These excitations have a larger gap and carry the same quantum numbers as the kinks of the SO(8) spectrum [9]. The cooperon is no longer a stable excitation in the large $U/t$ limit, but becomes instead a diffusive state made of these two kinks. One thus expects that the gap ratio $\Delta_1/\Delta_c$ saturates at 1/2 in the SO(6) regime, in full agreement with the numerical results of Fig. 2. The physics of the strong-coupling regime can also be investigated by a complementary approach: to map directly, in the large $U$ limit, the SU(4) Hubbard model (1) onto a SU(4) AFM Heisenberg chain by a standard perturbation theory in $t/U$ [11]: $\mathcal{H}_{\rm eff} = J \sum_i S_i \cdot S_{i+1}$, with $J = 4t^2/U$ and $S_i^A$ are SU(4) spin which belongs to the six-dimensional representation of SU(4). This SO(6) AFM Heisenberg chain is not integrable and has been studied by means of the density matrix RG approach [11]. In full agreement with our results, this model belongs to a SU(4) dimerized phase. Using the numerical results of Ref. [11], we find that our QMC results for the spin gap $\Delta_s(U/t)$ follow a SO(6) Heisenberg regime for $U > 8t$. In this respect, we deduce that the low-energy physics of the SO(6) AFM Heisenberg chain is described by the six almost free massive Majorana fermions (5).

*Crossover regime.*—Both SO(8) and SO(6) regimes differ by the coherent nature of spin-orbital excitations and the existence of an elementary charge $2e$ cooperon excitation. In the simplest hypothesis, the crossover between these two regimes can be understood as a change of sign of the coupling $G_s$ as a function of $U$. A mean-field analysis of the low-energy effective theory together with our numerical results predict that such a crossover occurs at $U \simeq 4.5t$ [9]. When $G_s(U) > 0$, the Majorana fermions of Eq. (5) experience an attractive interaction, and the neutral bound state in the adjoint representation of SU(4) are formed. The latter excitation is adiabatically connected to one of the bosonic states of the SO(8) spectrum, which is responsible of the sharp peak in the dynamical structure factor in the SO(8) regime. It is thus very tempting to conclude, within this simple scenario, that the SO(8) regime approximately extends up to $U_c \sim 4.5t$, above which one enters the Heisenberg SO(6) regime.

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