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Effective Theory of Magnetization Plateaux in the Shastry-Sutherland Lattice

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We use the nonperturbative Contractor-Renormalization method (CORE) in order to derive an effective model for triplet excitations on the Shastry-Sutherland lattice. For strong enough magnetic fields, various magnetization plateaux are observed, e.g., at $1/8$, $1/4$, $1/3$ of the saturation, as found experimentally in a related compound. Moreover, other stable plateaux are found at $1/9$, $1/6$, or $2/9$. We give a critical review of previous works and try to resolve some apparent inconsistencies between various theoretical approaches.

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The Shastry-Sutherland lattice [1] and its realization in the material $\text{SrCu}_2(\text{BO}_3)_2$ have been attracting a lot of attention due to its fascinating behavior in a magnetic field [2–4], namely, that magnetization plateaux have experimentally been observed for values of $m = 1/8$, $1/4$, and $1/3$ of the saturation value. The Shastry-Sutherland lattice, sketched in Fig. 1(a), is a two-dimensional (2D) Heisenberg antiferromagnetic spin-1/2 coupled-dimer system which Hamiltonian reads

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z. \quad (1)$$

Experiments with $\text{SrCu}_2(\text{BO}_3)_2$ indicate that the ratio between inter- and intradimer coupling should be close to $J'/J \approx 0.65$ where the ground-state is exactly given by the product of singlets on J bonds [5]. In the presence of a finite magnetic field h , polarized triplets are created on the dimer bonds so that low-energy properties can be described with an effective model of these “particles”: since these triplets are hard-core bosons moving on an effective square lattice, they can typically exhibit compressible superfluid or incompressible Mott phases depending on the filling [5,6]. In the original language, these two phases correspond, respectively, to absence or presence of magnetization plateaux.

In order to provide a simple picture, let us recall that the triplet hopping is strongly reduced on frustrated lattices, and therefore, the physics is governed by effective Coulomb repulsion, resulting in various insulating phases known as Wigner crystals. Following these pioneering works, other theoretical approaches have confirmed the occurrence of several plateaux [5,7]. While all approaches agree to describe $m = 1/2$ or $1/3$ plateaux, the situation is less clear at lower magnetization.

Experimentally, because of accessible fields, the first plateaux were discovered at $1/8$ and $1/4$ [3], but recently, translation symmetry breaking has been observed above $1/8$ [8,9] as well as evidence of $1/6$ plateau [10]. By using torque measurements, Sebastian *et al.* [11] have suggested additional magnetization plateaux for more “exotic” val-

ues like $1/9$, $1/7$, $1/6$, $1/5$, and $2/9$. Although an agreement on these values has not been reached yet, these results are quite exciting and ask for a thorough theoretical analysis.

Because of the lack of powerful numerical techniques or unbiased analytical tools to tackle 2D frustrated systems, a promising approach consists in deriving an effective hardcore bosonic model. Because one is interested in low-magnetization (i.e., low filling), long-range effective interactions are crucially needed and can only be captured thanks to efficient algorithms. Recently, perturbative continuous unitary transformations up to high orders have provided such an effective model [12]. In this Letter, we use the *nonperturbative* Contractor Renormalization (CORE) technique [13,14] in order to derive an effective model for the polarized triplets. Then, in order to provide an unbiased analysis of this model, we solve it *exactly* on various clusters and by finite-size scaling analysis, we predict the existence or not of some plateaux in the thermodynamical limit.

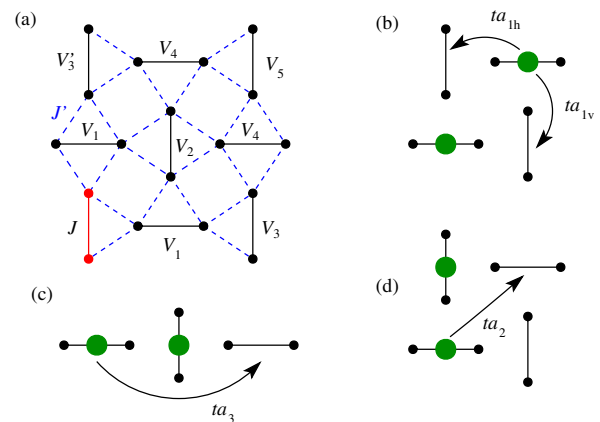


FIG. 1 (color online). Shastry-Sutherland lattice and definitions of some effective interactions: (a) 2-body interaction between a particle on the bottom left dimer and one on the labeled dimers. (b)–(d) Typical correlated hopping processes.

Effective model.—Similar to perturbation theory [5,6], we base our approach on keeping only the singlet and polarized triplet states on each dimer [15]. A crucial aspect of the CORE technique is that it gives a cluster expansion of the effective Hamiltonian \mathcal{H}_{eff} . Basically, the amplitude of local processes can already be captured by solving a small finite cluster. As a consequence, the only approximation consists in truncating beyond a certain range of interactions [13]. In our study, we keep *all* processes that can appear on a 3×3 cluster (corresponding to 18 original sites). Note that some elementary processes, as nearest-neighbor repulsion or chemical potential, are already well captured with a smaller 2×2 cluster so that different truncations may give similar amplitudes. Nevertheless, long-range interactions are crucially needed to describe low-filling phases. Typically, \mathcal{H}_{eff} contains of the order of 10^4 terms, similar to what is obtained with high-order perturbation [12].

Our CORE calculation gives access to the chemical potential μ which corresponds to the spin gap. As sketched in Fig. 2(a), CORE results are in good agreement with 4th order perturbation theory [5] up to $J'/J = 0.7$. Because of the important role played by diagonal 2-body interactions, we compare them with high-order perturbation theory [12] in Fig. 2(a). Clearly, these interactions decrease with distance and are nonisotropic: for instance, V_3 and V'_3 strongly

differ. Generally, one also notices very good agreement between perturbation theory (third order [5,6] or higher [12]) and CORE results at least up to values of $J'/J \approx 0.5$. Beyond this value, other processes become dominant so that comparison becomes more difficult to perform, and we will restrict to $J'/J \leq 0.5$ in our study.

Besides the discussed 2-body interaction terms, V_3^{3p} , that corresponds to an attractive interaction of three aligned particles, has a sizeable contribution (-0.7) close to $J'/J \sim 0.5$, quite different from high-order perturbation by Dorier *et al.* (-0.4). Although being high-order processes in perturbation, we believe that interaction terms involving three and more particles play an important role in the formation of plateaux. For example, in the one-dimensional realization of the Shastry-Sutherland lattice, namely, the orthogonal-dimer chain, diagonal interaction terms between several particles are responsible for the series of infinite plateaux [16].

The effective model also includes off-diagonal processes which account for hopping terms of bosons (i.e., triplets) from one dimer to another. In agreement with perturbation theory [6], we find that simple one-particle hopping terms are negligible. On the contrary, correlated hopping (i.e., when one-particle hops from one dimer to another in the presence of neighboring particle) is a dominant process, and we illustrate the three most important such terms in Fig. 1 and give the corresponding amplitudes in Fig. 2(b). Even though they may appear small, correlated hopping terms are very important for the physics of a system as they favor supersolid phases [17]. We note again a good agreement with perturbation theory up to $J'/J \approx 0.5$. Beyond that, as for diagonal terms, we observe strong variations of the amplitudes that indicate the limit of validity of our CORE truncation.

Validity of the CORE approach.—It is known that the physics of the Shastry-Sutherland model changes from a dimer state to a 2D-like Heisenberg phase above $(J'/J)_c \approx 0.70$, possibly with an intermediate plaquette phase [5]. Naturally, the question of the validity of our CORE approach emerges. In this regime, we observe that (i) basic processes amplitudes do not converge with different cluster sizes; (ii) ground-state has zero overlap with our subspace. Therefore, CORE procedure is only applicable below this critical value.

Another useful tool to ascertain the validity of CORE approach is to compute exactly on small clusters the reduced density matrix weights of retained states [14]. A numerical analysis done on 16-site cluster confirms that the total weight of the 2 kept states exceeds 85% as long as $J'/J \leq 0.65$. This gives us confidence that effective interactions should decay fast enough so that our CORE procedure is accurate in this region. Because of the reduced accuracy close to this J'/J value [which describes the $\text{SrCu}_2(\text{BO}_3)_2$ compound], we will restrict most of our findings to $J'/J = 0.5$ where various CORE truncations

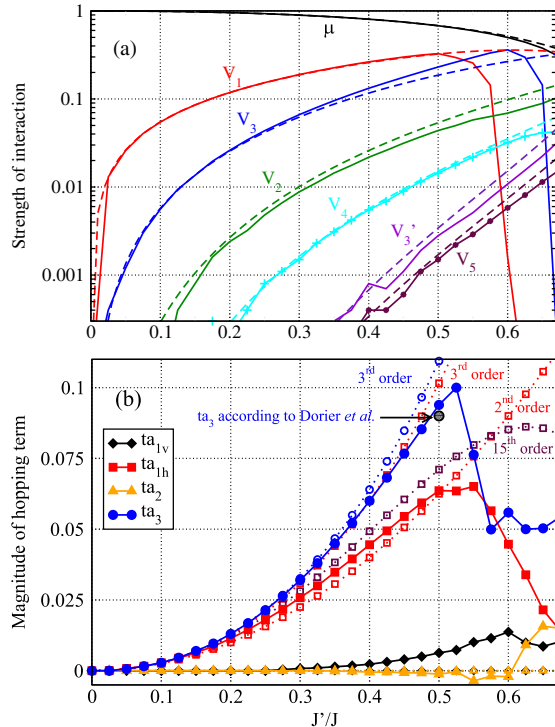


FIG. 2 (color online). Effective amplitudes, defined in Fig. 1, calculated with CORE (solid lines) and perturbation theory (dashed lines, see text): (a) μ and 2-body diagonal terms; (b) correlated hoppings and high-order perturbation result for ta_{1h} and ta_3 from Dorier *et al.* (private communication).

give similar models. Still, this value is reasonably close to the experimental one, and no qualitative changes are expected in this region. In particular, the same magnetization plateaux should occur.

In all these effective models approaches, one must distinguish the two steps: first, an effective Hamiltonian is derived; then, because it is still an interacting quantum problem, one needs to resort to an efficient technique to study it. Although it is a bosonic model, the presence of positive off-diagonal terms prohibits quantum Monte Carlo calculations. Possible alternatives are mean-field analysis [12] which main drawback is to overestimate the tendency to form plateaux and also needs a careful numerical analysis on finite clusters. Given the various small amplitudes, we prefer not to make any further assumption, and we provide *exact diagonalizations* (ED) of these effective models on finite lattices.

Simulations of the effective model.—By solving exactly the effective models for various bosonic fillings, it is straightforward to construct the magnetization curve by a Legendre transform. A typical plot is given in Fig. 3(a) where we compare data obtained with the microscopic and effective models on $N = 32$ lattice. Because a given finite

lattice cannot accommodate all magnetization values (only multiples of $2/N$ are allowed), the magnetization curve presents many steps. Thus, we cannot conclude yet about the existence of other plateaux, such as $1/6$, and one needs to do a careful finite-size extrapolation to get information on the thermodynamical limit.

Nevertheless, for this system size, Fig. 3(b) shows that our effective Hamiltonian is extremely accurate, as it remarkably coincides with exact values (both for plateaux widths and locations) at least for magnetization $m \leq 0.5$. Moreover, this accuracy is excellent up to $J'/J \sim 0.4$, and we only observe a small disagreement for $m = 1/2$ and $J'/J = 0.5$. A huge advantage of our effective model is that, although it involves many terms (basically, all terms up to 9-body), due to Hilbert space reduction, we are able to solve systems twice as large as for the microscopic model, which makes feasible a finite-size scaling. We have therefore solved \mathcal{H}_{eff} on a $N = 64$ lattice, and its magnetization curve is given in Fig. 3(a). Naturally, there are twice as many finite-size steps, but the main message is that $m = 1/4$ and $m = 1/8$ plateaux *do not change*, both in sizes and locations. This strongly suggests that our model does exhibit magnetization plateaux in the thermodynamical limit. Because we have chosen particular clusters, there is also the possibility to have more stable plateaux close to these fractions, and for instance, some plateaux that we find could be unstable towards phase separation.

Other possible fractions can be investigated by performing similar calculations with other square clusters, like $N = 36$ and 72 , that can also accommodate $m = 1/9$, $1/6$, $2/9$, and $1/3$. Data are shown in Figs. 3(c) and 3(d) and confirm (i) the accuracy of our CORE effective model and (ii) the stability of some plateaux when the system size is doubled, strongly indicating that they do persist in the thermodynamical limit.

In order to give a general view of various fractions, we now turn to a more systematic study of our effective Hamiltonian, restricted to the typical $J'/J = 0.5$ value, on various square or rectangular clusters. By computing the magnetization curves on several lattices, we can perform a finite-size scaling of the plateaux widths (see Fig. 4). Note that we restrict our calculations to clusters that can accommodate a given insulating phase, i.e., are not frustrated, according to the known patterns [3,5]. Since we also have access to density-density correlations, we can also confirm these patterns (data not shown): for instance, at $m = 1/3$ (resp. $m = 1/4$), the plateau is formed by filled diagonal stripes separated by two (resp. three) empty ones.

Our scaling provides clear evidence that there are large plateaux for $m = 1/3$ and $1/4$ (besides $m = 0$ and $1/2$) in the thermodynamical limit [18]. Moreover, within the very good accuracy of our effective model, finite-size scaling indicates smaller, but stable, plateaux for $2/9$, $1/6$, $1/8$, and $1/9$ of typical sizes between $0.01J$ and $0.05J$.

Discussion.—By allowing for inhomogeneous patterns, a variety of fractions have been found theoretically [11,12].

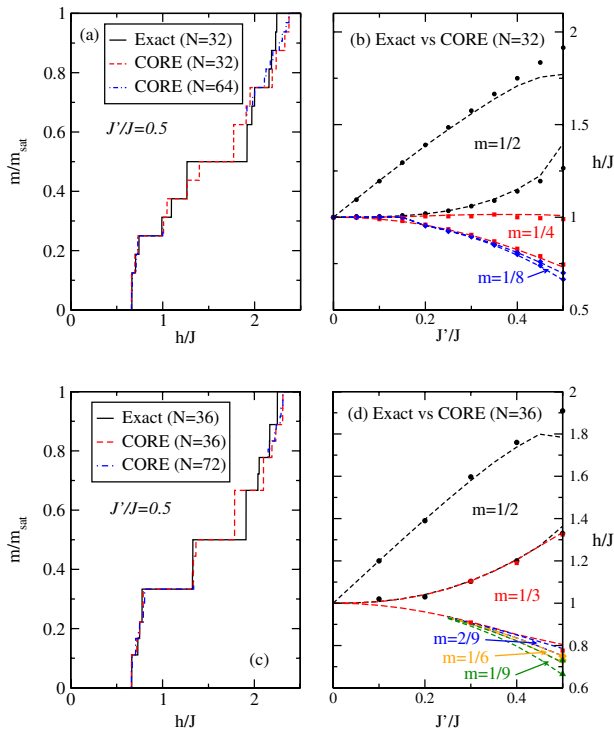


FIG. 3 (color online). (a) Magnetization curve obtained with microscopic and CORE models on $N = 32$ lattice and CORE results on 64-site for $J'/J = 0.5$. (b) Phase diagram for $N = 32$ as a function of J'/J and magnetic field h/J : CORE results (lines) agree with ED (symbols) for locations of $m = 1/2$, $1/4$, and $1/8$ plateaux which are allowed on this cluster. (c), (d) Same as (a), (b) for $N = 36$ and 72 . On these clusters, $m = 1/2$, $1/3$, $1/6$, $1/9$, or $2/9$ plateaux are allowed.

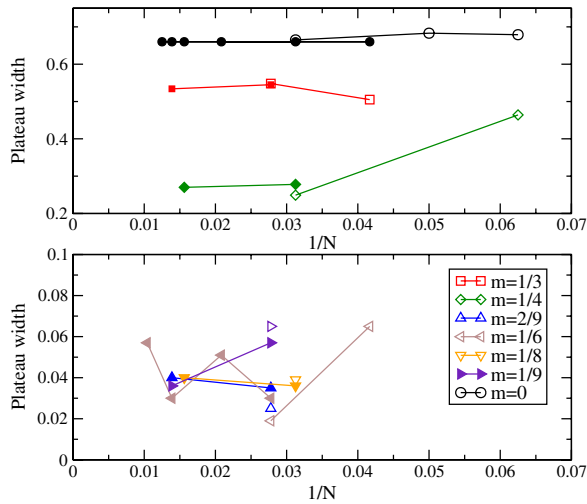


FIG. 4 (color online). Finite-size scaling of the plateau widths for various $m < 1/2$ from microscopic and CORE models (respectively, open and filled symbols) for $J'/J = 0.5$ on clusters with 24, 32, 36, 48, 64, 72, and 96 sites (square and rectangular). Note the excellent agreement between both models solved on the same lattices.

Experimentally, there is recent evidence that translation symmetry is broken for several other magnetization fractions [10,11]. Clearly, given the small energy scales that stabilize one fraction with respect to another, the accuracy of the calculation is crucial. In that sense, systematic perturbative [12] or CORE expansion (as in this Letter) are promising since they are controlled techniques. For instance, our relative error on the ground-state energy for $N = 32$ and $m = 1/8$ is 0.3%.

However, from these effective models, a second step is to solve them in the most unbiased way: here, we have combined exact diagonalization and finite-size scaling, and we find highly stable plateaux for $1/2$, $1/3$, $1/4$, but also smaller plateaux for $2/9$, $1/6$, $1/8$, and $1/9$. While some of these fractions coincide with [12], we also have some differences that ask for a clarification.

A first discrepancy is the absence in our data of plateaux for $m = 2/15$, observed in [12], or possible other fractions such as $1/7$ or $1/5$ found in [11]. Clearly, because our exact simulations are restricted to large but finite clusters, we cannot perform finite-size scaling for some fractions (as $2/15$ that would require large unit cells). By choosing adequate shapes or boundary conditions, it might be possible to investigate some of these other fractions.

A more crucial issue deals with $m = 1/4$ and $1/8$ plateaux that are stable in our calculations, and also found experimentally [2], but absent in [12]. A possible explanation could be that these fractions are unstable towards phase separation, but on our finite clusters, this phenomenon cannot be observed. However, these plateau widths are almost constant when the system size is doubled (see Fig. 4) so that we do strongly believe that they persist in the

thermodynamical limit. At this point, let us recall that our effective model is different from [12], in particular, for interactions with more than two bodies; for instance, if we only consider 2-body diagonal terms, then the $m = 1/4$ plateau becomes unstable, in agreement with [12]. Therefore, we think that many-body terms ask for a careful analysis.

As a conclusion, we are convinced that reliable effective Hamiltonians are crucial to understand the very rich low-magnetization properties of the Shastry-Sutherland system. With the CORE technique, we have derived such an effective model and, with finite-size scaling analysis, we provide a microscopic origin of the experimentally observed $1/3$, $1/4$, and $1/8$ plateaux, but we also confirm the possibility of other plateaux at $1/9$, $1/6$, and $2/9$, as found in recent related studies [10–12]. The remaining discrepancies between these approaches call for a systematic unbiased study that would combine mean-field ideas with exact diagonalizations.

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