Mechanisms for Spin-Supersolidity in $S = 1/2$ Spin-Dimer Antiferromagnets

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Using perturbative expansions and the Contractor Renormalization (CORE) algorithm, we obtain effective hard-core bosonic Hamiltonians describing the low-energy physics of $S = 1/2$ spin-dimer antiferromagnets known to display supersolid phases under an applied magnetic field. The resulting effective models are investigated by means of mean-field analysis and Quantum Monte Carlo simulations. A “leapfrog mechanism”, through means of which extra singlets delocalize in a checkerboard-solid environment via correlated hoppings, is unveiled that accounts for the supersolid behavior.

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I. INTRODUCTION

Concepts and techniques developed within a well established research field are often employed in exploring new physics displayed by apparently unrelated systems. Following this trend, there has been an increased interest in field-induced Bose-Einstein condensation of magnons in quantum magnets (for a recent review, see Ref. 1). Although the analogy is never complete, this line of research undoubtedly has led to considerable success in unveiling new phenomena in a growing number of magnetic insulators under applied magnetic field. The success of this approach suggests that one might be able to experimentally observe more elusive bosonic behavior in quantum magnets, such as the phase simultaneously displaying diagonal and off-diagonal order known as supersolid.

Supersolidity has attracted enormous interest since the detection of non-classical rotational inertia in solid Helium by Kim and Chan. 2 Although the correct interpretation of these measurements is still hotly debated and there seems to be no consensus on the possibility of supersolidity in translationally invariant systems, the occurrence of supersolid phases for bosonic models on a lattice is a well established fact. While the simplest model of interacting hard-core bosons on a square lattice is unstable against phase separation, which prevents supersolid behavior, it has been shown that frustration, removal of the hard-core constraint, or inclusion of generalized couplings in the Hamiltonian can stabilize supersolidity. Although a more direct implementation of these models remains elusive, due to the short ranged nature of interactions between atoms in optical lattices, one might expect that they are relevant in the context of quantum magnets under an applied magnetic field.

Indeed, as it was first shown by Ng and Lee and further verified by some of us, an $S = 1/2$ spin-dimer model on the square lattice with intra-plane coupling Ising-like anisotropy [see Eq. 1 below] has a phase simultaneously displaying diagonal and off-diagonal order, the equivalent of a supersolid for spin systems (henceforth dubbed spin-supersolid). Later spin-supersolidity was also shown to occur for $S = 1$ systems on a bilayer and on a chain. However, the exact relationship between these spin models and the aforementioned bosonic lattice models is not well understood. For instance, one might naively expect that the $S = 1/2$ spin-dimer model investigated in Refs. 18 and 19 will map onto a $t - V$ model for hard-core bosons on a square lattice, which is known not to display a supersolid phase. Therefore, in order to understand the mechanism behind supersolidity in this model one should analyze the presence of extra terms in the effective model.

Using a perturbative analysis and the contractor renormalization (CORE) method, we derive effective Hamiltonians for the $S = 1/2$ spin-dimer model studied in Refs. 18 and 19. A mean-field analysis of the resulting generalized hard-core bosonic Hamiltonian leads to a minimal model capable of accounting for supersolid behavior, which is then studied by means of Quantum Monte Carlo (QMC).

II. THE MODEL

We analyze the $S = 1/2$ spin-dimer Hamiltonian analyzed by Ng and Lee and some of us, which reads

$$\mathcal{H} = J_\perp \sum_i \vec{S}_{i,1} \cdot \vec{S}_{i,2} - h \sum_{i,\alpha} S_{i,\alpha}^z + J \sum_{\langle i,j \rangle, \alpha=1,2} \left( S_{i,\alpha}^x S_{j,\alpha}^x + S_{i,\alpha}^y S_{j,\alpha}^y + \Delta S_{i,\alpha}^z S_{j,\alpha}^z \right).$$

(1)

$\vec{S}_{i,\alpha}$ is an $S = 1/2$ operator attached to the site $i$ of the layer $\alpha$ (see Fig. 1). $J_\perp$ couples spins in different layers and is considered to be the essential coupling, being responsible for the system’s strong dimerized character (we set $J_\perp = 1$ throughout the rest of the paper).
the same layer interact via the coupling $J$ and $\Delta$ is an
Ising-like anisotropy; finally, the magnetic field $h$ is ap-
plied along the easy-axis. We will mainly focus on the set of
parameters considered in Refs. 18 and 19, $J/J_\perp = 0.29$
and $\Delta = 3.3$, leading to an extended supersolid phase as
evident from the QMC results for the spin stiffness $\rho_S$
and static structure factor $S(\pi, \pi)$ obtained by Lafforen-
cie and Mila20 and reproduced in Fig. 2

Our goal is to show that we can understand the emer-
gence of SS for the spin model Eq. (1) in terms of sim-
ple microscopic mechanisms. In achieving this, we de-
rive effective bosonic models for Eq. (1) by means of two
different procedures: high-order perturbative series ex-
pansions and the Contractor Renormalization algorithm
(CORE). We are going to show that correlated hoppings
for singlets (holes) with amplitudes $\tilde{s}_1$ (next-nearest-
neighbor, NNN, hopping which occurs only if at least one
of the other sites on the same plaquette is occupied) and
$\tilde{s}_2$ (assisted third-neighbor hopping occurring only when
the site in between is occupied), depicted in Fig. 3(a) and
(b) respectively, are crucial in accounting for SS behavior
for the model of Eq. (1). It is easy to see [Fig. 3(c)] that
these processes prevent phase separation in the hard-
core bosonic model on the square lattice ($t - V$ model)
by allowing extra singlets (holes) to delocalize in a checker-
board solid (CBS) environment by “leapfrogging” on the
other sublattice and forming a condensate. It is useful to
define the quantity we call “leapfrog ratio”

$$\Sigma = \frac{2|\tilde{s}_1| + |\tilde{s}_2|}{|\tilde{t}_1|},$$

where $\tilde{t}_1$ is the nearest-neighbor (NN) hopping amplitude
for holes. It was shown by Sengupta et al20 that the
energetic gain in the domain wall formation behind phase
separation in the $t - V$ model is $c\tilde{t}_1$, where $c$ lies in the
interval [1, 2]. Therefore, for a system of hard-core bosons
on the square lattice, the energetic gain associated to the
correlated hoppings depicted in Fig. 3 must be larger
than $c\tilde{t}_1$, implying that the condition $\Sigma > c/4$ must be
obeyed, for SS behavior to emerge.
III. PERTUBATIVE EXPANSIONS

Following the work of Totsuka and Mila we restrict ourselves to the limit where $J_{\perp}$ is the main energy scale and the system consists of weakly coupled dimers. The application of a magnetic field lowers the energy of one of the triplet bands and at the critical field $h_{c1}$ the singlet state $|s\rangle$ (holes) and the bottom of the triplet $|t^f\rangle$ (bosons) band become degenerate [see Fig. 1(b)]. By expanding the Hamiltonian Eq. (1) in terms of the small parameter $J/J_\perp$ we can thus obtain an effective hard-core bosonic model. Within first-order in $J/J_\perp$, the only effective couplings in the model obtained in this way are nearest-neighbor hopping amplitude $t_1$ and repulsion $V_1$ for the emergent bosons (triplets). However, since this so-called $t-V$ model [equivalent to Eq. (3) below if we set $s_{1,2}^P=0$] is known to display no SS phase,12 higher-order effective couplings should be taken into account and we proceed to their derivation.

A. Second-Order Expansion

We extend the perturbative analysis of Mila to second order in $J/J_\perp$, obtaining the following effective Hamiltonian

$$H_{\text{eff}}^{P^2} = -\mu^{P^2} \sum_i n_i + \sum_{(i,j)} \left[ t_1^{P^2} (b_i^\dagger b_j + \text{H.c.}) + V_1^{P^2} n_i n_j \right] + s_{1,2}^{P^2} \sum_{(i,j,k)} b_i^\dagger (1-n_j) b_k + \text{H.c.} ,$$

with effective couplings (we set $J_{\perp} = 1$)

$$\mu^{P^2} = 1 + \frac{J^2(2+\Delta^2)}{4} + \hat{h} ,$$

$$t_1^{P^2} = J/2 ,$$

$$V_1^{P^2} = \frac{J\Delta}{2} - \frac{J^2(2+\Delta^2)}{8} ,$$

$$s_{1,2}^{P^2} = 0.05$$

We have ignored constant terms and $\hat{\mu}^{P^2} = \mu^{P^2} + 2V_1^{P^2}$; $\hat{n}_i = b_i^\dagger b_i$ is now the singlet (holes) occupation number. In addition to the first-order couplings $t_1^{P^2}$ (NN hopping amplitude) and $V_1^{P^2}$ (NN repulsion) the second-order effective Hamiltonian also contains a correlated hopping term with amplitude $s_{1,2}^{P^2}$ [see Fig. 3(a-b)]. Correlated hoppings have been shown to stabilize supersolidity12 by allowing particles to delocalize in a CBS ordered background. However, the second-order amplitude for correlated hoppings is too small to prevent phase separation: the “leapfrog ratio” of Eq. (2) $\Sigma^{P^2} = 3J/8 \approx 0.12$ for $J/J_{\perp} = 0.29$ is too small and cannot account for supersolidity. Therefore we extend our analysis and include higher-order corrections to the parameters $t_1^{P^2}$, $V_1^{P^2}$ and $s_{1,2}^{P^2}$ in Eq. (3) with the help of perturbative continuous unitary transformations (PCUTs).
B. Perturbative Continuous Unitary Transformations (PCUTs)

The method of continuous unitary transformations (CUTs)\textsuperscript{25,26,27,28} in its perturbative variant\textsuperscript{29,30,31,32} and quasi-particle conserving form is an efficient tool to derive effective low-energy models for coupled quantum dimer networks in a magnetic field up to high order in perturbation\textsuperscript{33,34}.

To this end, the original spin Hamiltonian Eq. (1) is rewritten in terms of rung triplet operators $t_{\alpha}^{(l)}$ with $\alpha = \{\pm 1, 0\}$. This Hamiltonian does not conserve the number of triplets $|Q|$ and therefore the magnitude of $s_{2}^{P}$ is the relevant kinetic scale for supersolidity (a similar situation happens for the effective Hamiltonian derived from CORE, see Sec. IV A). As we mentioned before, supersolid behavior is expected to occur for large enough values of $s_{2}^{P}/t_{1}^{P}$\textsuperscript{16,17}. However, our results for this ratio, shown in the inset of Fig. [4], are clearly too small for preventing domain wall formation\textsuperscript{16,17} and therefore one does not expect to reproduce the extended SS phase observed for the original spin model, Eq. (1). Consequently, either our idea that the model can be described by only taking into account $|s\rangle$ and $|t\rangle$ is wrong, or we must go beyond a perturbative analysis. Since according to Ng and Lee\textsuperscript{48} contributions from the other two triplets states $|t^{+}\rangle$ and $|t^{-}\rangle$, if non-zero, are negligible close to half-filling, we therefore resort on a non-perturbative approach to our problem, namely the CORE algorithm.

IV. CONTRACTOR RENORMALIZATION

The contractor renormalization (CORE) method was introduced by Morningstar and Weinstein\textsuperscript{36,37} and has been recently\textsuperscript{35} applied to the study of the spin-dimer Hamiltonian described by Eq. (1). We extend these results by considering the next range in the effective couplings and analyzing in more detail the resulting effective bosonic model.

A. Procedure

The basic idea behind CORE (for comprehensive accounts the reader is referred to Refs. 39 and 40) is to project out high energy degrees of freedom and to derive an effective Hamiltonian describing the low-energy physics of the original model. Usually this is done by first decomposing the lattice on which the original model is defined into elementary blocks and diagonalizing the Hamiltonian on a single block (while an extended method without this restriction was introduced by some of us recently\textsuperscript{41} here the standard CORE method is more appropriate). After choosing a suitable number of low-energy block states, the model is subsequently diagonal-
ized on a cluster consisting of a few elementary blocks and the lowest energy cluster states are projected onto the restricted basis formed by the tensor products of the retained block states. An effective Hamiltonian is then obtained by imposing the constraint that the low-energy spectrum of the full problem is exactly reproduced and by subtracting shorter-range contributions obtained from previous steps involving lesser blocks. The validity of the procedure can be checked by either analyzing the magnitude of long-range effective couplings (large values associated to these signal the inadequacy of the chosen restricted set of degrees of freedom in accounting for the system’s low-energy behavior) or, perhaps more accurately, by keeping track of the weight of the reduced density-matrix associated to a single block.

For the spin-dimer model considered here, Eq. (1), large values for the inter-plane coupling $J_{\perp}$ imply that the natural choice when applying CORE is to consider the dimers as the elementary blocks: dimer singlet states, $|s\rangle$, corresponding to an unoccupied tensor in the effective model living on the square lattice, and an emergent boson created by promoting one singlet to an $S^z = 1$ triplet state, $|t\rangle$, are the retained block states. The adequacy of this reduced set of degrees of freedom in describing the Hamiltonian of Eq. (1) in the regime known to display supersolid behavior was verified by Abendschein and Capponi and is confirmed in the present work.

Our results are obtained from the analysis of the clusters depicted in Fig. 5. They are labelled according to the maximum range for the effective couplings: range-1 are the results obtained from the analysis of the cluster containing two dimers shown in Fig. 5(a), range-21/2 denote the ones from the cluster with four dimers arranged as a plaquette [Fig. 5(b)] and range-2 results from the three-dimer cluster shown in Fig. 5(c). We gauge the validity of the mapping onto a system of hard-core bosons by analyzing corrections to the nearest-neighbor (NN) hopping amplitude $t_1$ (for particles) obtained from range-21/2 and range-2 CORE calculations: whenever the sum of these contributions exceeds the value obtained from range-1 CORE we assume that a valid mapping is not obtained. While the criteria used by Abendschein and Capponi is probably more accurate, our results agree qualitatively with theirs and suffice for our analysis. More importantly, for the parameters ($\Delta = 3.3$ and $J/J_{\perp} = 0.29$) leading to supersolidity previously considered in the literature, both criteria validate the mapping onto the effective bosonic model.

The effective hard-core bosonic Hamiltonian obtained from the CORE calculation is, after applying a particle-hole transformation $(1 - n_i) \rightarrow \tilde{n}_i$ and $b^\dagger \rightarrow \tilde{b}_i$ given by

$$\mathcal{H}^C_{\text{eff}} = \sum_i \left\{ -\tilde{\mu}^C \tilde{n}_i + \left[ \tilde{V}_i + \tilde{W}_i \right] + \left[ \tilde{T}_i + \tilde{S}_i + \tilde{R}_i \right] \right\},$$

(8)

where $\tilde{\mu}^C$ is the chemical potential for the holes (singlets). $\tilde{V}$ comprises two-body interactions and $\tilde{W}$ three- and four-body interactions; $\tilde{T}$, $\tilde{S}$ and $\tilde{R}$ are the kinetic contributions; direct and correlated hopping terms. Full expressions for each of these terms are given in Appendix B.

B. Comparison with Pertubative Expansion

Figure 6 shows our results for the effective nearest-neighbor hopping amplitude $t_1$ (for particles) obtained from CORE (range-1, -21/2 and -2) and from PCUTs for $\Delta = 3.3$ and as a function of $J/J_{\perp}$. As expected, the various ranges CORE results agree with the ones obtained from PCUTs in the limit of small $J/J_{\perp}$, where both results are essentially exact. However, for $J/J_{\perp} \gtrsim 0.15$ higher-order terms in the perturbative expansion start to dominate, invalidating the PCUTs analysis. Crucially, for the value $J/J_{\perp} = 0.29$ considered in Refs. 18 and

![FIG. 6: (Color online) Comparison between CORE (range-1, -21/2 and -2) and PCUTs results for the nearest-neighbor hopping amplitude $t_1$ (for particles) in the effective bosonic model as a function of $J/J_{\perp}$ for $\Delta = 3.3$, as in Refs. 18 and 19. The value $J/J_{\perp} = 0.29$ is highlighted by the vertical dashed line. The vertical solid line indicates the point where longer range (21/2 and 2) corrections to $t_1$ become larger than the range-1 contribution, signaling the breakdown of the mapping onto a bosonic model (see main text).](image)
Table I: Couplings in the effective Hamiltonian obtained from CORE [up to range-2, Eqs. (8, B1-B5)] for $\Delta = 3.3$ and $J/J_\perp = 0.29$. Units are set by $J_\perp = 1$.

| $V_i^n$ | $W_i^n$ | $\tilde{V}_i^n$ | $\tilde{W}_i^n$ |
|--------|--------|----------------|----------------|
| 0.336874 | -0.011122 | -0.008851 | 0.009035 |
| -0.002257 | -0.009378 | 0.000988 | -0.008850 |

(19) (highlighted by the vertical dashed line Fig. 4), the PCUTs expansion is clearly invalid, while longer-range CORE results are essentially converged.

These results can be understood if we remark that any perturbative expansion about the weakly coupled dimer limit is only valid as long as one stays in the zero-field rung-singlet phase, with a finite gap to all three triplet modes. However, it has been shown\textsuperscript{18,19} that for $\Delta = 3.3$ and $J/J_\perp = 0.29$ the zero-field ground-state of the spin-dimer model Eq. (1) displays long-range Néel order implying the existence of a quantum critical point $J_s/(h = 0)/J_\perp < 0.29$ (evident from poles in Padé analysis for the perturbation series) beyond which our perturbative expansions become meaningless. On the other hand, although CORE relies on a strong dimerized character (so that dimer singlets and triplets are the relevant local degrees of freedom), it does not assume any particular ordering and therefore remains valid across the critical regime.

V. MECHANISM FOR SPIN-SUPERSOLIDITY

Numerical values obtained from CORE for all effective couplings (up to range-2) appearing in Eqs. (8, B1-B5) are shown in Table I for the parameters $\Delta = 3.3$, $J/J_\perp = 0.29$ used in the original QMC simulations.\textsuperscript{18,19}

We use the mean-field (MF) approach discussed in Appendix C and calculate the dependence of the condensate density $\rho_0$ and CBS order parameter [see Eqs. (C4, C5)] on magnetic field $h$. The results are shown in Fig. 7a. The semi-quantitative agreement between these results and the QMC data for the original model Eq. (1) (shown in Fig. 8) is remarkable if we keep in mind that only contributions of up to range-2 have been considered in the CORE calculation. However, MF approaches are known to overestimate supersolid behavior,\textsuperscript{9,10,15} and the effects of quantum fluctuations must be carefully analyzed.

Unfortunately, the effective Hamiltonian obtained from CORE, Eqs. (8, B1-B5), is complex and poses great challenges for more unbiased analysis. We therefore use the aforementioned MF procedure in gauging the relative importance of each term, with a twofold purpose: (a) identifying the dominant mechanism accounting for supersolidity in the spin-dimer model of Eq. (1) and (b) obtaining a simpler effective model amenable to QMC simulations (see below) in order to check whether the conjectured mechanisms survive after quantum fluctuations are taken into account.

A. Minimal Hamiltonian

In deciding on a minimal model we should obviously take into account the magnitudes associated with each term in Eqs. (8, B1-B5). we start by neglecting all effective couplings smaller than $0.1\tilde{V}_C^0$, where $\tilde{V}_C^0$ is the NN hopping for holes (singlets). Furthermore, since SS takes place only close to half-filling, we can also neglect the four-body term with coupling $W_4^0$ [see Eq. (B2)]. The resulting model is identical to the second-order effective Hamiltonian [Eq. (6)], but with strongly renormalized couplings. In particular, the couplings associated to the correlated hoppings $V_2^C$ and $W_2^C$ [see Fig. 3 (a,b)] are considerably larger than predicted by the perturbative analysis\textsuperscript{24} as required for SS to emerge. However, the MF analysis of the resulting model shows that the extra kinetic energy associated to the large effective amplitudes for correlated hoppings requires the addition of the attractive two-body interactions $\tilde{V}_C$ and $\tilde{W}_C$ (see Table I) to stabilize a CBS plateau. These considerations lead...
to the minimal model:

\[ \tilde{H}_{\text{min}}^C = -\tilde{\mu}^C \sum_i \tilde{n}_i + \sum_{\langle i,j \rangle} \left[ \tilde{t}_1^C (\tilde{b}_i^\dagger \tilde{b}_j + \text{H.c.}) + \tilde{V}_2^C \tilde{n}_i \tilde{n}_j \right] + \sum_{\langle \langle i,k \rangle \rangle} \left[ \tilde{s}_1^C \left( \tilde{b}_i^\dagger (\tilde{n}_{j1} + \tilde{n}_{j2}) \tilde{b}_k + \text{H.c.} \right) + \tilde{V}_3^C \tilde{n}_i \tilde{n}_k \right] + \sum_{\langle \langle \langle i,l \rangle \rangle \rangle} \left[ \tilde{s}_2^C \left( \tilde{b}_i^\dagger \tilde{n}_l \tilde{b}_l + \text{H.c.} \right) + \tilde{V}_3^C \tilde{n}_i \tilde{n}_l \right]. \]  

(9)

\( \tilde{n}_i = \tilde{b}_i^\dagger \tilde{b}_i \) is the occupation number for holes; \( \langle i,j \rangle \), \( \langle \langle i,k \rangle \rangle \) and \( \langle \langle \langle i,l \rangle \rangle \rangle \) denote, respectively, NN, NNN and third-NN sites on the square lattice. The correlated hopping term with amplitude \( \tilde{s}_1^C \) [\( \tilde{s}_2^C \)] is depicted in Fig. 3(a) [Fig. 3(b)]: a hole hops between two NNN [third-NN] sites \( i \) and \( k \) [\( j \)] only if at least one of their common NN sites \( j_1 \), \( j_2 \) [\( j \)] is occupied by a hole. Mean-field results (not shown) for the superfluid density \( \rho_S \) and the CBS order parameter \( S(\pi, \pi) \) for the minimal model of Eq. (9), with effective couplings given in Table 1 (for \( \Delta = 3.3 \) and \( J/J_\perp = 0.29 \)), semi-quantitatively reproduce the QMC results (shown in Fig. 3) for the original spin-dimer model, Eq. (1). Unfortunately, this picture is too simplistic and results from QMC simulations (not shown) for this minimal model show that the CBS plateau is destroyed by quantum fluctuations, seemingly invalidating our analysis. However, the QMC results for \( S(\pi, \pi) \) display a rather pronounced peak, indicating that our minimal model is close to a borderline where the solid phase appears: this is confirmed by the existence of an extended CBS plateau (concomitantly with a SS phase) in the QMC results obtained by considering slightly smaller values for the NN hopping amplitude \( \tilde{t}_1^C \), suggesting that terms neglected in the full effective model [Eqs. (8) to (13)], although relatively small, play an important role.

A closer examination of the terms in the full effective CORE Hamiltonian [Eqs. (8) to (13)] neglected in deriving our minimal model Eq. (9) shows that the NN correlated hoppings with amplitudes \( \tilde{s}_3^C \) and \( \tilde{s}_5^C \) [see Eq. (13)] and Table 1 have exactly the effect of decreasing the holes’ (singlets’) kinetic energy that may stabilize the CBS phase. However, the fact that \( \tilde{t}_1^C \) and \( \tilde{s}_3^C \), \( \tilde{s}_5^C \) have opposite signs also implies that their inclusion in Eq. (9) has the undesired effect that the resulting minimal model would suffer from the sign problem. In order to circumvent this problem and be able to perform QMC simulations, we incorporate \( \tilde{s}_3^C \) and \( \tilde{s}_5^C \) in an effective way: we notice that in a perfectly ordered CBS background these extra hoppings effectively reduce the NN hopping amplitude \( \tilde{t}_1^C \) to the value we denote \( \tilde{t}_1^\text{min} \) given by (to leading order)

\[ \tilde{t}_1^\text{min} = \tilde{t}_1^C - (|\tilde{s}_3^C| + |\tilde{s}_5^C|). \]

(10)

MF results [Fig. 7(b)] for the new minimal effective model obtained by the substitution \( \tilde{t}_1^C \rightarrow \tilde{t}_1^\text{min} \) in Eq. (9) suggests that the dominant physical processes are correctly taken into account, at least close to half-filling, as we can conclude from the excellent agreement with the results for the full effective CORE model [Fig. 7(a)]. Furthermore, the SS region visible in Fig. 7(b) is expected to survive quantum fluctuations, for a sizable lepap ratio \( \Sigma(\tilde{t}_1^\text{min}) \approx 0.43 \) is obtained for \( \Delta = 3.3 \) and \( J/J_\perp = 0.29 \), something confirmed by our QMC simulations below.

B. Quantum Monte Carlo Simulations

We have performed QMC simulations, using an extended version of the ALPS libraries’ implementation of the Stochastic Series Expansion (SSE) algorithm. We consider the minimal effective model of Eq. (9) with NN hopping amplitude \( \tilde{t}_1^\text{min} \) given by Eq. (10). We evaluate the superfluid density \( \rho_S \), obtained in terms of the winding numbers \( w_x \) and \( w_y \)

\[ \rho_S = \frac{1}{2\beta L^2} \left( w_x^2 + w_y^2 \right), \]

(11)

where \( \beta \) is the inverse temperature and \( L \) is the system size, and the CBS order parameter

\[ S(\pi, \pi) = \frac{1}{L^2} \sum_{\vec{r}_i,\vec{r}_j} (-1)^{\vec{r}_i-\vec{r}_j} \tilde{n}_{\vec{r}_i} \tilde{n}_{\vec{r}_j}, \]

(12)

as a function of the magnetic field \( h \). Since we are interested in accessing ground-state properties, and the main kinetic energy scale in the minimal model Eq. (9) is \( \tilde{t}_1^\text{min}/J_\perp \approx 0.13 \), we set the temperature to \( T = 1/20L < 0.5 \).
\[ \tilde{\rho}_{\text{min}}^4 / 2L. \] It is important to remark that these temperatures are considerably lower than those considered by Ng and Lee, who assumed that \( J / J_1 = 0.29 \) was the relevant energy scale, and this might explain the round shape observed in some of their curves.

QMC results for \( \rho_S \) and \( S(\pi, \pi) \) for the minimal model of Eq. (11) with NN hopping amplitude given by Eq. (10), using the effective couplings appearing in Table I (\( \Delta = 3.3 \) and \( J / J_1 = 0.29 \)), are shown in Fig. 8. The overall agreement with QMC results for the original spin-dimer model Eq. (1) shown in Fig. 2 is good and we can conclude that the minimal model of Eqs. (9) and (10) indeed accurately describes the low-energy physics of the original model and, more importantly, that the “leapfrog mechanism” presented in Sec. II is at least partially responsible for spin-supersolid behavior.

Although the just presented results show that the essential ingredients for spin-supersolidity have been identified, it is clear that quantitative agreement is not achieved. Specifically, the extent of the SS phase is considerably smaller in Fig. 8 than in Fig. 2; reversely, the CBS phase in the former is about twice as large than in the latter. In trying to understand this mismatch it is important to keep in mind that supersolidity emerges in this model as the result of a delicate balance between kinetic and interaction terms. This is evident in the MF analysis discussed in Sec. IV A which suggests that the effective model obtained from CORE is close to a border-line and that small variations in the effective couplings can have drastic effects. For instance, we have shown that the minimal model Eq. (9), with effective couplings shown in Table II does not display a CBS phase; however, by replacing \( \tilde{C}_1 \rightarrow \tilde{\rho}_{\text{min}}^4 \) [Eq. (10)] we obtain a CBS phase twice as large as expected.

Therefore, and since the sign-problem precludes us from performing QMC simulations for the full effective Hamiltonian [Eqs. (9) and (10)], we conjecture that that terms ignored in obtaining the minimal model [Eqs. (9) and (10)], even with small couplings, must be included in order to better reproduce the results for the original model, shown in Fig. 2. Additionally, the NN correlated hoppings with amplitudes \( \tilde{s}_{ij}^\perp \) and \( \tilde{s}_{ij}^\parallel \) appear to favor SS and the fact that we include only their effects in reducing \( \tilde{C}_1 \) [Eq. (10)] might be responsible for the reduced SS phase in Fig. 8. Finally, it is not possible to exclude the possibility that longer range effective interactions and/or neglected triplet excitations \((|t^{0}\rangle, |t^{-1}\rangle)\) may be required for obtaining quantitative agreement.

C. Extent of the Supersolid Phase

We have extended our MF analysis to the full effective model Eqs. (9) and (10) by varying the parameters \( \Delta \) and \( J / J_1 \), as a function of the magnetic field \( h \). Results are shown in Fig. 9. Grey shaded areas represent values of \( \Delta \) and \( J / J_1 \) for which no SS phase is stabilized within MF for all values of \( h \) and only a superfluid and/or CBS phases are obtained. However, SS does appear over an extended region in the parameters space within MF.

![Fig. 9: (Color online) Successive phases stabilized for increasing magnetic field \( h \) in the parameter space of the spin-dimer model of Eq. (1), as obtained from a mean-field analysis of the full CORE Hamiltonian, Eqs. (9) and (10).](image)

CBS phases are obtained. However, SS does appear over an extended region in the parameters space within MF. Since it is well known that MF tends to overestimate supersolidity, we have also analyzed the “leapfrog ratio” \( \Sigma(t_{\text{min}}^4) / \Sigma(t_{\text{min}}^4) \) throughout the parameters space. As discussed in Sec. III the condition \( \Sigma(t_{\text{min}}^4) / \Sigma(t_{\text{min}}^4) > c / 4 \), with \( c \in [1, 2] \), must be satisfied for preventing phase separation and stabilizing a SS. Regions for which this condition is fulfilled are indicated in Fig. 9. We can see that the region where the SS phase is likely to occur is much smaller than expected from the MF analysis and, in particular, no SS is expected within the perturbative limit.

VI. CONCLUSIONS AND OUTLOOK

Summarizing, we have obtained effective models describing the low-energy physics of a spin-dimer model [Eq. (11)] known to exhibit spin-supersolid behavior, with the help of perturbative expansions and of the contractor renormalization (CORE) algorithm. While the perturbative analysis, relying on the assumption of a disordered ground state with gapped excitations at zero-field, does not reproduce the extended supersolid phase observed in the original model (Fig. 2), CORE does not assume any particular ordering in the system and is
shown to reproduce the main features obtained from more computationally demanding approaches, even when a simple mean-field procedure is applied to the obtained effective model.

Furthermore, we identify the mechanism at play behind spin-supersolidity and we show that the spin-supersolid phase exhibited by the $S = 1/2$ spin-dimer model of Eq. (1) can be simply understood in terms of the “leapfrog mechanism” illustrated in Fig. 5. Basically, a sizable amplitude for correlated hoppings allow extra holes (singlets) to delocalize on the other sublattice of a checkerboard solid, preventing phase separation and leading to supersolid behavior.

More generally speaking, we are able to describe the physics behind complex phenomena in a simple way by deriving effective models with only a few terms and rather local couplings. The essential physical ingredients can be identified even in a low-order perturbative analysis, although more sophisticated approaches, such as PCUTs and CORE, may be required in obtaining the effective couplings. We highlight that both PCUTs and CORE are immune to the sign problem and can therefore be applied to frustrated and fermionic systems, something which opens interesting research possibilities.

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APPENDIX A: PCUTS SIXTH-ORDER EFFECTIVE COUPLINGS

The effective couplings obtained from the PCUTs analysis discussed in Sec. II B are

$$V^P_1 = \frac{1}{2} J \Delta - \frac{3}{16} J^2 \Delta^2 - \frac{13}{32} J^3 \Delta - \frac{1}{16} J^4 \Delta^3 + \frac{79}{128} J^5 \Delta^2 - \frac{95}{1024} J^6 \Delta$$

$$t^P_1 = \frac{1}{2} J - \frac{1}{4} J^2 - \frac{3}{8} J^3 \Delta^2 - \frac{13}{32} J^4 \Delta - \frac{1}{16} J^5 \Delta^3$$

APPENDIX B: EFFECTIVE COUPLINGS FROM CORE

The explicit expressions for each term in the effective Hamiltonian obtained from CORE, Eq. (S), are given here (in the expressions below $\tilde{n}_i = \tilde{b}_i^\dagger \tilde{b}_i$ is the occupation number for holes and $\tilde{x}, \tilde{y}$ are unity vectors for the square lattice; constant terms arising from applying a particle-hole transformation to the bare CORE effective Hamiltonian are ignored). $\tilde{V}$ comprises two-body interactions

$$\tilde{V}_1 = \tilde{V}^{\tilde{C}}_1 (\tilde{n}_i \tilde{n}_{i+\hat{x}} + \tilde{n}_i \tilde{n}_{i+\hat{y}}) + \tilde{V}^{\tilde{C}}_2 (\tilde{n}_i \tilde{n}_{i+\hat{x}+\hat{y}} + \tilde{n}_i \tilde{n}_{i+\hat{x}-\hat{y}}) + \tilde{V}^{\tilde{C}}_3 (\tilde{n}_i \tilde{n}_{i+2\hat{x}} + \tilde{n}_i \tilde{n}_{i+2\hat{y}})$$

and $\tilde{W}$ three- and four-body interactions

$$\tilde{W}_1 = \tilde{W}^{\tilde{C}}_1 (\tilde{n}_i \tilde{n}_{i+\hat{x}} \tilde{n}_{i+\hat{y}} + \tilde{n}_i \tilde{n}_{i+\hat{y}} \tilde{n}_{i+\hat{x}}) + \tilde{W}^{\tilde{C}}_2 [\tilde{n}_i \tilde{n}_{i+\hat{x}} (\tilde{n}_{i+\hat{y}} + \tilde{n}_{i+\hat{x}+\hat{y}} + \tilde{n}_{i-\hat{y}} + \tilde{n}_{i+\hat{x}-\hat{y}})] + \tilde{W}^{\tilde{C}}_3 (\tilde{n}_i \tilde{n}_{i+\hat{x}} \tilde{n}_{i+\hat{y}} \tilde{n}_{i+\hat{z}} + \tilde{n}_i \tilde{n}_{i+\hat{z}} \tilde{n}_{i+\hat{y}}).$$

The effective single-boson hopping terms in Eq. (S) are

$$\tilde{t}_1 = \tilde{t}^{\tilde{C}}_1 (\tilde{b}_i \tilde{b}_{i+\hat{x}} + \tilde{b}_i \tilde{b}_{i+\hat{y}} + \text{H.c.}) + \tilde{t}^{\tilde{C}}_2 (\tilde{b}_i \tilde{b}_{i+\hat{x}+\hat{y}} + \tilde{b}_i \tilde{b}_{i+\hat{x}-\hat{y}} + \text{H.c.})$$
Correlated hopping terms are

\[ \hat{S}_i = \hat{S}_i^C \left[ \hat{b}_i^\dagger (\hat{n}_{i+x} + \hat{n}_{i+y}) \hat{b}_{i+x+y} + \hat{b}_i (\hat{n}_{i-x} + \hat{n}_{i-y}) \hat{b}_{i-x-y} + \text{H.c.} \right] + \hat{b}_i^\dagger \hat{b}_{i+x}\hat{b}_{i+x+y} \hat{b}_{i-y} + \text{H.c.} \]

and, finally, hoppings simultaneously involving two-bosons

\[ \hat{R}_i = r_i^\phi \left( \hat{b}_i^\dagger \hat{b}_{i+x+y} + \hat{b}_i \hat{b}_{i-x-y} + \hat{b}_i \hat{b}_{i+y} \right) + \hat{b}_i^\dagger \hat{b}_{i+y} \hat{b}_{i-x-y} + \text{H.c.} \]

\begin{equation}
\text{APPENDIX C: MEAN-FIELD PROCEDURE}
\end{equation}

Following the Matsubara-Matsuda semiclassical approach, we write the hard-core boson effective models in terms of \( S = 1/2 \) pseudo-spin variables. We start by replacing the commutation relations for bosons on the same site \( i \),

\[ [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0 \quad \text{and} \quad [b_i, b_j^\dagger] = 1 \quad (C1) \]

by the fermionic anticommutation relations

\[ \{b_i, b_j\} = \{b_i^\dagger, b_j^\dagger\} = 0 \quad \text{and} \quad \{b_i, b_j^\dagger\} = 1 \quad (C2) \]

while retaining the canonical bosonic commutators for operators on different sites \( i, j \). This leads to an algebra formally equivalent to that of a spin 1/2.

We then neglect quantum fluctuations by replacing the pseudo-spin operators by their mean value, obtaining a Hamiltonian in terms of classical spins variables

\[ \mathcal{S} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta) \] which reads

\[ \mathcal{H}_{MF} = h_{\text{eff}} \sum_i S_i^z + (\sum_{i,j} \left[ J_{ij}^z S_i^z S_j^z + J_{ij}^x S_i^x S_j^x + S_i^y S_j^y \right] + \sum_{(i,j,k)} \left[ K_{ijkl}^z S_i^z S_j^z S_k^z + S_i^y S_j^y S_k^y \right] + \sum_{(i,j,k,l)} [M_{ijkl}^z (S_i^z S_j^z S_k^z S_l^z) + \text{H.c.}] \] (C3)

The parameters \( h_{\text{eff}} \) (one-body), \( J \) (two-body), \( K \) (three-body), \( L \) (four-body) and \( M \) (double exchange) are defined in terms of the couplings in the effective bosonic Hamiltonian. The superscript \( z (\perp) \) accounts for interactions (hoppings) between sites coupled as in the bosonic Hamiltonian.

In accounting for the different phases of the Hamiltonian Eq. (i) it suffices to consider a site-factorized wavefunction \( |\psi\rangle = \prod_i |\psi_i\rangle \) assuming two-sublattice long-range order \( (i = A, B) \). The variational parameters \( (\phi_A, \phi_B, \theta_A \text{ and } \theta_B) \) are determined by minimizing the ground-state energy per site within this subspace. The condensate density corresponds in a MF approach to the magnetization in the \( xy \) plane

\[ \rho_0 = \frac{1}{8} (\sin^2 \theta_A + \sin^2 \theta_B) \quad (C4) \]

and the CBS structure factor is

\[ S(\pi, \pi) = (\cos \theta_A - \cos \theta_B)^2 / 4 \quad (C5) \]

In terms of the density of singlets in the sublattice \( A \), given by

\[ n_A = \frac{1 + \cos \theta_A}{2} \quad (C6) \]

with a similar definition for the sublattice \( B \) \( (n_B) \), the ground state energy per site \( E_0 \) (up to a constant) for the minimal model of Eqs. (9)(10).

\[ E_0 = 2 \tilde{V}_i^C n_{AB} n_B + (\tilde{V}_3^C + \tilde{V}_d^C) (n_A^2 + n_B^2) + 4 \tilde{V}_c^C \sqrt{n_A (1 - n_A)} \sqrt{n_B (1 - n_B)} \cos (\phi_A - \phi_B) + 2 (\tilde{s}_x^C + 2 \tilde{s}_y^C) n_{AB} (2 - n_B - n_A) + \left( h - \mu \right) \frac{n_A + n_B}{2} \quad (C7) \]

We can therefore deduce the following trends:
Due to the sign of $\tilde{V}_C^1$, $\tilde{V}_C^2$ and $\tilde{V}_C^3$, the terms of Eq. (C7) and Eq. (C8) favor the CBS because in order to minimize them, one must break $A - B$ symmetry (cf. Fig. 10(b)).

On the contrary, the kinetic term Eq. (C9) (cf. Fig. 10(a)) favors the SF phase: it is indeed minimal for $n_A = n_B$ and $\phi_A - \phi_B = \pi$. There is then no symmetry breaking between $A$ and $B$ sublattices and the latter relation introduces an order in the $xy$ plane confirming the presence of a SS phase.

The last term Eq. (C10) is more subtle. In the case where $\tilde{s}_C^1$ and $\tilde{s}_C^2$ are negative as presently, the contribution of Eq. (C10) does not break the translational symmetry and therefore only favors the SF phase. But it is yet sufficient to induce a SS as shown on Fig. 10(c). This figure shows that the minimization of the total MF energy indeed leads to translational symmetry breaking ($n_A \neq n_B$) but as the highest density of both is not equal to one, we do not obtain a CBS phase but the SS one. What is not shown is that minimizing $E_0$ also leads to $\phi_A - \phi_B = \pi$ or in other words to an order in the $xy$ plane which is the semiclassical equivalent of the condensate density.

For the sake of completeness, let’s mention that if we would have considered the contributions of $\tilde{s}_C^3$ and $\tilde{s}_C^5$ indirectly inserted in the minimal Hamiltonian due to the sign problem, they would have led to an MF energy...
In order to minimize it, $\phi_A - \phi_B$ must be equal either to 0 or to $\pi$ which introduces an order in the $xy$ plane. Moreover, if $\phi_A - \phi_B = \pi$ (as actually imposed by Eq. (10), it also leads to a breaking of the $A-B$ symmetry as shown by Fig. (10) (c). At the MF level, this correlated hopping term alone favors both symmetry breakings contrary to Eq. (10).

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48. By reducing $C_1$ from the starting value 0.145 and keeping all the other couplings appearing in Eq. (1) unchanged, CBS and SS already appear for $C_1 \sim 0.14$.
49. A MF analysis for the enlarged minimal model including, besides terms appearing in Eq. (1), the correlated hopping terms with amplitudes $s_C^C$ and $s_C^C$ [Eq. (13)], reveals an enlarged SS region (compared with the one obtained for the full effective model). This suggests that the terms with amplitudes $s_C^C$ and $s_C^C$ play a role in stabilizing SS and the fact that they are not explicitly included in the minimal model Eq. (1) might explain the shrunk SS region in our QMC results.
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