Extended supersolid phase of frustrated hard-core bosons on a triangular lattice

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We study a model of hard-core bosons with frustrated nearest-neighbor hopping \((t)\) and repulsion \((V)\) on the triangular lattice. We argue for a supersolid ground state in the large repulsion \((V \gg |t|)\) limit where a dimer representation applies, by constructing a unitary mapping to the well understood unfrustrated hopping case. This generalized ‘Marshall sign rule’ allows us to establish the precise nature of the supersolid order by utilizing a recently proposed dimer variational wavefunction, whose correlations can be efficiently calculated using the Grassman approach. By continuity, a supersolid is predicted over the wide parameter range, \(V > -2t > 0\). This also establishes a simple phase diagram for the triangular lattice spin 1/2 XXZ antiferromagnet.

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Supersolidity, where superfluid and crystalline orders coexist, have fascinated physicists since they were first theoretically proposed\(^{[1]}\). Recent experimental results in \(^4\)He\(^{[2]}\) that are still under active debate have led to renewed interest. Experimental developments on a different front, in the realization of optical lattices in ultracold atomic systems, motivated a search for a lattice supersolid. One of the more promising candidates is a model of strongly interaction hard-core bosons on a triangular lattice. The model Hamiltonian reads

\[
H = -i \sum_{\langle ij \rangle} (b^*_i b_j + \text{H.c.}) + V \sum_{\langle ij \rangle} \left( n_i - \frac{1}{2} \right) \left( n_j - \frac{1}{2} \right),
\]

where \(b_i (b^*_i)\) annihilates (creates) a hard-core boson on site \(i\) and \(n_i = b^*_i b_i\) are density operators. The model is equivalent to the XXZ spin-1/2 Hamiltonian on the triangular lattice

\[
H = \sum_{\langle ij \rangle} \left[ \frac{J_z}{2} (s^+_i s^-_j + s^-_i s^+_j) + \frac{J_s}{4} s^y_i s^y_j \right],
\]

where \(s^\pm = (1/2)(s^x \pm is^y), s^x,y,z\) are the Pauli matrices and are related to bosons by \(s^\pm = (2n_{i} - 1), s^+ = b^\dagger, s^- = b,\) and \(J_z = V, J_s = -2t\). The discussion below will be largely in terms of the bosons, although we will sometimes switch to the equivalent spin description, when that is more natural. The \(t > 0\) case corresponds to the unfrustrated hard-core boson model with repulsive nearest-neighbor interactions. For this case, a variety of studies including large scale quantum Monte Carlo simulations\(^{[3,4,5]}\) indicate a supersolid phase for all \(V/t \geq 8.9\), stabilized by an ‘order by disorder’ mechanism. The solid order is of the three sublattice \((+++)\) type, where two sublattices have the same boson density.

The case of frustrated hopping \((t < 0)\) suffers from a sign problem in the occupation number basis, and its ground state has been a subject of conjecture for the last three decades. The corresponding spin model is just the XXZ antiferromagnet, which, in the large \(J_z\) limit was at the center of the RVB spin liquid proposal of Fazekas and Anderson\(^{[6]}\). Later semiclassical and small cluster numerical studies suggested magnetic order\(^{[7]}\), and general arguments which apply to the phase structure of bipartite dimer models, to which this model can be mapped in the large \(J_z\) limit, also indicate the same result\(^{[8,9]}\). However, the precise nature of ordering has not been conclusively established. In this letter, we show how this problem can be tackled, which is summarized briefly in boson language below. Due to frustration, the ground states in the \(V \to \infty\) limit is extensively degenerate. Within this ground state manifold, we demonstrate that the frustrated problem with \(t < 0\) can be mapped, via a nontrivial unitary transformation, onto the unfrustrated one with \(t > 0\). Since the latter is well understood\(^{[3,4,5,10]}\), many properties of the frustrated case can be immediately derived. Such a generalized ‘Marshall sign’ was conjectured earlier based on state enumeration and numerics\(^{[6,11]}\). Here we construct the explicit transformation which proves this conjecture, and moreover utilize it to deduce properties of the frustrated model. Our unitary transformation is diagonal in the occupation number basis, which, combined with our knowledge of the unfrustrated model, allows us to argue that a supersolid state is realized for \(t < 0\) as well. The precise details of the superfluid phase ordering requires further calculation. This is carried out using a variational wave-function approach\(^{[12]}\) recently introduced for the unfrustrated \(t/V = 0^+\) limit, which captures the essential aspects of supersolid order very well and has good variational energy as compared to the quantum Monte Carlo results. Applying the unitary transformation, we obtain a variation wave-function for the frustrated problem. Properties of this wavefunction, in particular the phase correlations, are then calculated. The state is found to be a supersolid and the resulting structure of the long range order (LRO) is shown in FIG. 4. Surprisingly, the superfluid amplitude vanishes on one of the sublattices and hence superfluidity lives exclusively on the honeycomb lattice formed by the remaining two sublattices, on which the amplitude alternates in sign. Contrary to naive expectations, the superfluid amplitude on these sites exceeds the maximum superfluid amplitude of the unfrustrated case.

Finally, with this information in hand, we propose a phase diagram for the entire \(t/V > 0\) parameter range. Note the point \(t/V = 1/2\) corresponds to the spin-isotropic triangular antiferromagnet, where the 120º state is established. This can be smoothly connected to the large \(V\) supersolid state derived here as shown in FIG. 1. Supersolid order would
then naturally be preserved over the wide parameter range $0 < -t < V/2$, in contrast to the unfrustrated case, where it is only present for $t < V/10$. The frustrated triangular lattice boson model therefore appears to be an appealing candidate for the realization of the elusive supersolid phase - experimental prospects are discussed at the end. Note, this is also a phase diagram for the spin 1/2 XXZ magnet, and the regime of proposed RVB phase of Fazekas-Anderson is actually a particular spin ordered state.

**Strong Repulsion Limit and Generalized Marshall Sign:** In the limit of $V \gg |t|$, we can restrict the Hilbert space to a manifold of states which correspond to classical Ising ground states of the triangular antiferromagnet. Every such Ising configurations $S$ can be represented by a close-packed dimer configuration $C$ on the dual honeycomb lattice. This is a two-to-one mapping because of the Ising $Z_2$ symmetry (particle-hole symmetry in the boson language). The Hamiltonian, projected into this degenerate subspace, introduces dynamics which splits the degeneracy. Note, to first order in degenerate perturbation theory, only the hopping term $H_t = -t \sum_{(i,j)} (b_i b_j + H.c.)$ plays a role, leading to the double-hexagon resonance in FIG. 2(a) with amplitude $-t$. The problem of the large repulsion limit is therefore related to finding the ground state of a quantum dimer model with such dimer resonances. We have already noted that the $t > 0$ case is tractable by Quantum Monte Carlo methods since there is no sign problem. However, the problem of interest here is the case $t < 0$. If there is a unitary transformation which changes the sign of every matrix element of $H_t$, the problem can be mapped to unfrustrated case. This is generically not possible but, within the restricted Hilbert space, this indeed happens, and the required unitary transformation is the following. Consider the lattice in FIG. 2(c) with 1/4 special edges marked as thick and green. One can check by inspection that any double-hexagon resonance will change the number of covered special edges by $\pm 2$. Therefore, if we define a unitary transformation on the dimer basis

$$|C'\rangle = U|C\rangle = e^{N_s(C)}|C\rangle,$$

where $i = \sqrt{-1}$, and $N_s(C)$ is the number of special (green) edges covered by a dimer in the dimer configuration $C$, the sign of the Hamiltonian will be changed. The unitary transformation does not change the energy spectrum nor correlations that are diagonal in boson density. Hence, thermodynamics - that only depends on energy eigenvalues- is unchanged, for eg. transition temperature and nature of transitions. However, off-diagonal correlations are affected. We can therefore immediately conclude that the ground state has the same three sublattice density modulation as the supersolid phase in the unfrustrated model. Moreover, it also has a finite compressibility, identical to that in the unfrustrated problem, since this can also be expressed as a density-density correlation function. The latter strongly suggests superfluid long range order (a 2D bosonic phase with finite compressibility at zero temperature), and taken all together this points towards supersolid order for $t/V = 0^-$ as well. In order to directly establish off diagonal long range order, and obtain more detailed quantitative information, we turn to a variational wavefunction approach.

**Variational Wavefunction** We denote the two Ising states related to the dimer state $C$ as $S[C]$ and $\bar{S}[C]$ and consider the following kind of wavefunctions,

$$|\Psi\rangle = \sum_{C} \phi(C) |C\rangle = \sum_{C} \phi(C) \cdot (|S[C]\rangle + |\bar{S}[C]\rangle) / \sqrt{2}$$

where $\phi(C)$ is the (complex) amplitude. In the dimer representation, the projected $H_t$ corresponds to the double-hexagon resonance in FIG. 2(a). Only those dimer configurations with ‘resonatable’ double hexagons appear in the Hamiltonian matrix elements. We denote by $c_{ij}$, that a particular dimer covering has a resonatable double hexagon at the pair of adjacent plaquettes $i, j$, where $i$ is the plaquette with two dimers. Under resonance $c_{ij} \rightarrow \bar{c}_{ij} = c_{ji}$. However, the rest of the dimer configuration with this pair of plaquettes removed $d_{ij}$ remains unchanged. Hence, the entire dimer configuration may be denoted as $c_{ij} + d_{ij}$. Note, a single dimer configuration may

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**FIG. 1:** Schematic phase diagram for both unfrustrated ($t > 0$) and frustrated hopping ($t < 0$) with repulsive interactions ($V > 0$). The three arrows are order parameters $s = (b_i+b_i, i b_i - i b_i, 2n - 1)$ on the three sub-lattices. For $t/V < -1/2$ or $t/V > 0.1$ there is only superfluid LRO (XY spin order). The thick line $-1/2 < t/V < 0.1$ is the region of supersolid order. $t/V = -1/2$ is the SU(2) symmetric antiferromagnet.

**FIG. 2:** (Color online) (a): two double-hexagon resonance configurations $c_{ij}$ and $\bar{c}_{ij} = c_{ji}$. Red thick bars denote dimers. (b): Kasteleyn orientation and edge weights of the honeycomb lattice. Thick blue edges have weight $z$, others have weight 1. The green dash-line rhombus encloses the enlarged unit cell. $x,y$ are the principal axis. We use the six sites on a thick-edge hexagon as the basis, labeled as $1, \ldots, 6$ as shown in the right-bottom corner. (c): special edges (thick green on the honeycomb) for the unitary transformation relating the unfrustrated and frustrated case. Thin solid green bonds on the triangular lattice are dual to the special edges.
have many representations in this notation - one for each res-
onsable hexagon pair. The variational energy $E = \langle \Psi | H_t | \Psi \rangle$ is

$$E = -t \sum_{<ij>} \sum_{d_{ij}} [\phi^* (c_{ij} + d_{ij}) \phi (\bar{c}_{ij} + d_{ij}) + c.c.]$$  \hspace{1cm} (5)$$

where c.c. is the complex conjugate. Before considering the
frustrated case in detail, we briefly review the variational
wavefunction for the unfrustrated case [12]. There, $t > 0$, so
the matrix elements of $H_t$ are all non-positive in the
dimer basis. Thus the Perron-Frobenius theorem applies and the
ground state can be taken to be everywhere positive. Hence,
we get a normalizable wavefunction if $\phi (C) = \sqrt{P(C)}$ with
$P(C)$ taken as the probability of the dimer configuration $C$.
Equivalently, one can assign positive weights $W(C)$ to each
dimer configuration $C$, then the probability $P(C) = W(C)/Z$,
where $Z = \sum C W(C)$.

The central assumption that leads to tractable wavefunc-
tions is the following. We assign weight $w_{ab}$ to all hon-
eycomb lattice edges $ab$, and write the weight of dimer cover-
ing $C$ as $W(C) = \prod_{\text{covered}} (ab) w_{ab}$. Interpreting $W$ as a ficti-
cious Gibbs weight, this corresponds to a problem of hardcore
dimers in an external potential. Powerful Grassmann variable
Techniques have been developed for this problem, which will
allow us to calculate properties of these wavefunctions.

Plug the ansatz $\phi (C) = \sqrt{P(C)}$ into (5), and using the fact
that the ratio $\frac{P(c_{ij} + d_{ij})}{P(c_{ij})}$ is independent of the configuration $d_{ij}$.

$$E = -t \sum_{<ij>} \sqrt{P(c_{ij})} P(\bar{c}_{ij})$$  \hspace{1cm} (6)$$

where $P(c_{ij}) = \sum d_{ij} P(c_{ij} + d_{ij})$ is the net probability of the
local configuration.

The dimer number operator is $n_{ab} = (1 + s_i^x s_j^z)/2$ where $ab$
is the honeycomb lattice edge dual to the triangular lattice
edge $ij$. The probability $P(c_{ij})$, $P(\bar{c}_{ij})$ are the expectation
values $\langle \psi_{1234567890} | n_{ab} \psi_{1234567890} \rangle$, $\langle \psi_{1234567890} | n_{ab} \psi_{1234567890} \rangle$, respec-
tively. This can be evaluated analytically by the Grass-
mannian integral method [14]. In the Grassmannian formu-
lation, the dimer partition function is represented as an integral
over Grassmannian variables $\eta_a$ defined on the honeycomb
lattice sites, $Z = \int \exp \left( \sum_{a,b} \eta_a a_{ab} \eta_b / 2 \right) \prod_a \eta_a = Pf[A]$, where $Pf[A]$ is the Pfaffian of the Kasteleyn
matrix $A$ [15], and $A_{ab} = +w_{ab}$ if the Kasteleyn orientation is from $a$
to $b$, or $= -w_{ab}$ if otherwise (see FIG. 2 (b)). The prob-
ability $P(c_{ij})$ is calculated as an expectation value in the
Grassmannian theory, the rule is to replace $n_{ab}$ by $A_{ab} \eta_a \eta_b$, then we get $P(c_{ij}) = w_{12} w_{34} w_{56} w_{78} w_{90} \langle \prod_{a=1}^{10} \eta_a \rangle$. Thus the variational energy (6) can be written as $E = -t \sum_{<ij>} \sqrt{\prod_{a=1}^{10} w_{i_a+i_j}} \langle \prod_{a=1}^{10} \eta_a \rangle$ with $w_{10,11} = w_{10,11}$. The ten-point correlator of anticommuting $\eta$ can be Wick-
expanded into a Pfaffian of a $10 \times 10$ antisymmetric matrix,
$\langle \prod_{a=1}^{10} \eta_a \rangle = Pf[\eta_a \eta_b] = \sqrt{\det[\eta_a \eta_b]}$, $a, b = 1 \ldots 10$. The above formula can be further simplified to the
determinant of a $5 \times 5$ matrix exploiting the bipartiteness of the
honeycomb lattice: $\langle \prod_{a=1}^{10} \eta_a \rangle = \det[\eta_a \eta_b]$, $a = 1, 3, \ldots, 9; b = 2, 4, \ldots, 10$. This is much more effi-
cient than the brutal-force Wick expansion used by Sen et al.
[12], which allows us to evaluate more complicated cor-
relation functions later in this paper. The two-point correlator $\langle \eta_a \eta_b \rangle = (A^{-1})_{ab}$ can now be evaluated by a Fourier
transformation since the Kasteleyn matrix $A$ has 2D translational
symmetry. For the chosen Kasteleyn orientation and basis
shown in FIG. 2 (b)), in the thermodynamic limit, the two-
point correlator of the site $a$ in unit cell $(0,0)$ and the site $b$ in
unit cell $(x,y)$ is

$$\langle \eta_a(x,0) \eta_b(x,y) \rangle = \int_0^{2\pi} \int_0^{2\pi} \langle A^{-1} \rangle_{ab} e^{i(k_x x + k_y y) \frac{dk_x dk_y}{4\pi^2}}$$

where $a, b = 1, \ldots, 6$, and $A^{-1}$ is the inverse of the $6 \times 6$
anti-hermitian matrix $A$.

$$\langle A \rangle \equiv \left( \begin{array}{ccc} 0 & 3 & x \\ -R \mid x & 0 & 3 \\ x & 3 & 0 \end{array} \right)$$

with $R(\bar{k}_x \bar{k}_y) = (1 - \epsilon_x \bar{k}_x \bar{k}_y)$, $\epsilon_x = e^{i k_x}$,
$\epsilon_y = e^{i k_y}$. As is shown in Ref. 12 for $t > 0$ this variational wavefunction has two local minima
at $z \approx 0.9258$ with energy per site $E = -0.13774t$, and
$z \approx 1.073$ with energy per site $E = -0.13762t$, corre-
sponding to the two supersolid states, $(+ - -)$ and $(0 + -)$ of
the triangular lattice boson model [2, 4, 5]. For the frustrated
case, the wavefunction is obtained by unitary transformation,
$|\Psi'\rangle = U |\Psi\rangle = \sum C \phi(C) |C\rangle$, hence the variational
wavefunction is $\phi(C) = i N_C \sqrt{P(C)}$. The variational energy
$E = \langle \Psi' | H_t | \Psi' \rangle$ is of course the same as in the unfrustrated
case. In order to understand the two variational wavefunctions
better, we shall calculate two point correlation functions, as-
suming for simplicity that the two points $i, j$ are on the same
horizontal line, and $j$ is on the right.

**Diagonal Correlations:** Consider first the density-density
correlation function $\langle s_i^x s_j^x \rangle$. Draw a line from $i$ to $j$ and
it will cut through an set of honeycomb lattice edges $< ab >$. If
the number of edges with no dimers cut by this line is even, then
$s_i^x s_j^x = +1$ and otherwise $= -1$. In terms of the dimer num-
ber operator $n_{ab}$ the $s_i^x s_j^x$ becomes a non-local string operator,

$$\langle s_i^x s_j^x \rangle = \prod_{<ab> \text{ cut by } ij} (2n_{ab} - 1) \hspace{1cm} (7)$$

Expand the product we get $2^{j-i}$ terms, $|j - i|$ is the distance
between $j$ and $i$ measured by the triangular lattice constant,
each of which is the type of correlation functions evaluated
before. Because these operators are diagonal in the dimer ba-
sis, $\langle s_i^x s_j^x \rangle = \langle s_i^x \rangle \langle s_j^x \rangle$. $\langle s_i^x \rangle = \langle s_j^x \rangle$.

**Off-diagonal Correlations:** The square of the off-diagonal
long range order (ODLRO) parameter $\langle b_i^\dagger b_j \rangle$ is slightly more
complicated. In the dimer basis it describes the simultane-
ous resonances of two hexagons (if $i$ and $j$ are not neighbors).
However for this process to happen $s_i^z$ and $s_j^z$ must be opposite. Label the two local resonating configurations on hexagon $i(j)$ by $C_{i(j)}$ and $C_{i(j)}^{\perp}$, there are two possibilities of this simultaneous double-resonance, shown in FIG. 3 with opposite conditions for the edges cut by the line $i + x$, $j - x$, where $x$ is the horizontal triangular lattice vector. The even(odd) requirement can be enforced using the dimer number operators as $[1 + \prod(2n_{ab} - 1)]/2$, where the product is over all edges $<ab>$ cut by the line $i + x$, $j - x$ (see FIG. 3 for an example). Consider $t > 0$ case first, we have

$$\langle \hat{\Psi}|b_i\rangle = \frac{\prod w}{(2n_{ab} - 1)!/2} \left[ \sum_{a=1}^{12} w_{a} \right] \eta_{a}$$

(8)

where the $\prod w$ is the product of edge weights of the twelve(12) edges around hexagons $i$ and $j$. Note, this simple form arises because the string $\prod(2n_{ab} - 1)$ cancels out. We will see shortly that in the frustrated hopping case, this does not happen.

If distance between $i$ and $j$ is large, the 12-point correlator $\langle \prod_{a=1}^{12} \eta_{a} \rangle$ can be factorized into two 6-point correlators $\langle \prod_{a=1}^{6} \eta_{a} \rangle$. And we have the relation $\sqrt{\prod w_{a=1}^{12}} = \langle \hat{\Psi}|b_i\rangle |\hat{\Psi}\rangle$. So literally we have the factorization property

$$\langle \hat{\Psi}|b_i\rangle \rightarrow \langle \hat{\Psi}|b_i\rangle |\hat{\Psi}\rangle |\hat{\Psi}\rangle, \quad |j - i| \rightarrow \infty$$

For $t < 0$ case we need to take care of the phases of $\phi'$. From FIG. 3(c) we can see that $\langle \hat{\Psi}|b_i\rangle |\hat{\Psi}\rangle$ has similar form as the first line of (8), only the first term inside $\{ \cdot \}$ acquires a minus sign. Therefore we get

$$\langle \hat{\Psi}|b_i\rangle |\hat{\Psi}\rangle = -\frac{\prod w}{(2n_{ab} - 1)!/2} \left[ \sum_{a=1}^{12} w_{a} \right] \eta_{a}$$

(9)

The product can be expanded into $2^{j-i-2}$ terms, each of which can be evaluated as before. Note, this correlation function cannot be factorized as in the unfrustrated case and one necessarily needs to evaluate a string correlator.

**Results:** We evaluate the above mentioned correlators up to distance $|j - i| = 18$ and extrapolate to infinite distance limit to determine the long range order.

At the global energy minimum $z = 0.9258$ and for the unfrustrated ($t > 0$) case, the long range order parameter $\langle \hat{s} \rangle = \langle \hat{b}^\dagger + b, ib - ib^\dagger, 2n - 1 \rangle = (0.163, 0.764), (0.372, 0, -0.412), (0.372, 0, -0.412)$ for the three sublattices A, B, and C, respectively (we have set the superfluid phase to zero and sublattice A is surrounded by weight $z$ hexagon in FIG. 2(b)). These numbers are in agreement with Quantum Monte Carlo (QMC) results. The average density deviation from 1/2 is $|0.764 - 0.412 - 0.412|/2 = 0.10$, which is about 2%, in good agreement with QMC [4]. The solid order parameter is $|n_A + n_B e^{2\pi i/3} + n_C e^{4\pi i/3}|/2 = 0.0384$ (n_A, B, C are boson densities on the three sublattices), which is about 15% smaller than the QMC result of 0.045 [4, 10], but in good agreement with classical Monte Carlo calculations result 0.0389 of the same type of variational wavefunctions [12].

In the frustrated ($t < 0$) case the three sublattice order parameter is $(0, 0, 0.764), (0.389, 0, -0.412), (-0.389, 0, -0.412)$, as shown in FIG. 4. The average density deviates from 1/2 by the same amount as the frustrated case. In spin language this means a non-zero average z-component of spin, $|\sum_i s_i^z/N| = |\sum_i s_i^z/(2N)| = 0.01$, which is about 50% smaller than harmonic spin-wave result 0.02, which has the same symmetry [4]. Note that surprisingly the superfluid amplitude ($XY$-component of $\hat{s}$) on the B, C sublattices is larger than those in the unfrustrated case, while it vanishes on the A sublattice. Note, this quantity can be directly measured in Quantum Monte Carlo simulations of the unfrustrated system in the large repulsion limit, by calculating correlations of the unitarily transformed operator. For example, with $O = s_i^x s_j^x$, with $j$ to the right of $i$ in the same horizontal line and $|j - i| > 2$, the correlator to be measured is $U^4 O = -s_j^x s_i^x s_j^x (2n_{ab} - 1)$. Finally, we combine the present
results in the large repulsion (or $V \gg -t$) limit with known $120^\circ$ order in the isotropic $V = -2t$ ($J_z = J_\perp$) limit. These can be connected without a phase transition, is we assume that the supersolid phase persists with no change in symmetry over the entire range $V > -2t > 0$. This scenario, which is also a phase diagram for the spin 1/2 XXZ antiferromagnet, is depicted in Figure[17][18]

**Experimental Realization:** How can the frustrated boson hoppings be experimentally realized? In lattice cold atom systems, a recent experiment [16] demonstrated that ‘repulsively’ bound molecular bosons have frustrated hoppings. Consider preparing an initial state composed of molecules of pairs of atoms (either bosons or fermions) with one or zero molecules per site. If the interactions between atoms are now made repulsive, the effective molecular hopping is readily seen to be frustrated, since the singly occupied sites are lower in energy. If this metastable state is sufficiently long lived, the equilibrium properties of the frustrated boson system can be accessed. In Josephson Junction Arrays, external magnetic fields can generate frustrated hopping[17].

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