Frustration-induced supersolids in the absence of inter-site interactions

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We discuss a novel mechanism for the realization of supersolids in lattices in the absence of inter-site interactions that surprisingly works as well at unit filling. This mechanism, that we study for the case of the sawtooth lattice, is based on the existence of frustrated and un-frustrated plaquettes. For sufficiently large interactions and frustration the particles gather preferably at un-frustrated plaquettes breaking spontaneously translational invariance, resulting in a supersolid. We show that for the sawtooth lattice the supersolid exists for a large region of parameters for densities above half-filling. Our results open a new feasible path for realizing supersolids in existing ultra-cold atomic gases in optical lattices without the need of long-range interactions.

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I. INTRODUCTION

Supersolids have attracted a large interest since they were proposed\cite{1,2} due to their, apparently counter-intuitive, co-existence of both crystalline order and superfluidity. Superfluidity on top of the crystalline order is explained by the creation and delocalization of zero point defects (such as vacancies or interstitials) in a strongly interacting system. The search for the elusive supersolid remains a challenge\cite{3,4}. The claimed evidence of supersolidity in Helium\cite{5}, was subsequently explained by the shear modulus stiffening of solid $^4$He\cite{6,7}.

Supersolidity may occur as well in lattices due to inter-site interactions. Lattice supersolidity has attracted an active theoretical interest as well\cite{8,9}. Ultra-cold gases in optical lattices provide an interesting system for the realization of lattice supersolids. However, the requirement of sufficiently large inter-site interactions reduces the possible scenarios for supersolidity to gases with long-range interactions, including dipolar gas\cite{10,11} and Rydberg–dressed atomic gases\cite{12,13}. These systems present however difficulties due to inelastic collisions in polar molecules\cite{14} and short life times in Rydberg gases.

An alternative to polar gases is provided by experiments with condensates in optical cavities, where infinitely long-range interactions between the condensed atoms are induced by two-photon processes. These interactions drive the Dicke phase transition that results in self-organized supersolids\cite{15}. Although these experiments are realized in absence of optical lattices, the self-organized supersolids break spontaneously a discrete spatial symmetry, hence resembling the case of lattice supersolids.

Long-range interactions are however not necessary for the realization of lattice supersolids. Recent studies on frustrated lattices with flat bands, such as kagome lattices\cite{16} and Creutz ladder\cite{17,18}, have discussed the possibility of observing supersolids without inter-site interactions. In the case of the Creutz ladder, supersolidity at incommensurate densities results from effective next-to-nearest neighbor hopping in the vicinity of the two flat band region, and the doping of a Valence Bond Crystal.

In this paper we discuss a novel mechanism that leads to robust lattice supersolidity in the absence of inter-site interactions. The mechanism is based on the existence of frustrated and un-frustrated plaquettes. In this sense, although we study the specific case of a sawtooth lattice, we expect that supersolids may be also realized in other lattice geometries fulfilling this property. Supersolidity follows from the preferential occupation of un-frustrated plaquettes, which results in spontaneously broken translational symmetry. Sawtooth lattices and other frustrated geometries may be realized using lattice shaking\cite{19} and similar laser arrangements as those recently employed for creating variable lattice geometries\cite{20,21}. Hence our results open a new feasible path for realizing supersolidity in existing atomic gases without the need of long-range interactions.

The structure of the paper is as follows. In Sec. II we introduce the sawtooth model studied in the paper. Section III discusses the non-interacting regime. Section IV is devoted to the ground state phase diagram, both at unit-filling and away from unit filling. In Sec. V we introduce a simple model that allows an intuitive understanding of the super solid mechanism. Section VI discusses the roton instability responsible for the superfluid-to-supersolid transition. In Sec. VII we comment on the experimental realization of the sawtooth model, and on the signatures of the supersolid phase. Finally, we summarize our conclusions in Sec. VIII.
The system is described by the Bose-Hubbard model (BHM): hence constitute two distinct sublattices, which we denote as A and B. For a sufficiently deep lattice, the system is described by the Bose-Hubbard model (BHM):

\[ \mathcal{H} = -t \sum_i (a_i^\dagger b_i + b_i^\dagger a_{i+1}) + \text{H.c.} \]

\[ + t' \sum_i (a_i^\dagger a_{i+1} + \text{H.c.}) + \frac{U}{2} \sum_{\nu \in \{A,B\}, i} n_i^\nu (n_i^{\nu *} - 1) \]

where \( a_i^\dagger \) and \( a_i \) are creation and annihilation operators for bosons at site \( i \) of leg A (B), and \( n_i^\nu = a_i^\dagger a_i \). \( n_i^2 = b_i^\dagger b_i \) is the number operator at site \( i \) of leg A (B). Contact-like interactions lead to the on-site interaction term, characterized by the coupling constant \( U \). Henceforth we consider all the physical quantities in units of \( t = 1 \) which makes them dimensionless.

### III. NON-INTERACTING REGIME

At first, it is convenient to study the non-interacting regime \((U = 0)\). In that case Model (1) may be diagonalized in momentum \((k)\) space (note that due to the broken sublattice symmetry, \( k \in [-\pi/2, \pi/2) \)): \[ \mathcal{H} = \sum_{\alpha, \beta} [E_\alpha(k) a_k^\dagger \alpha_k + E_\beta(k) b_k^\dagger \beta_k], \]

where the first \((\alpha)\) and second \((\beta)\) energy bands are characterized by the dispersion \( E_\alpha, \beta(k) = -t' \cos 2k \mp 2t' \cos k + (t'/t)^2 \cos^2 2k \)^{1/2}, and the bosonic operators \( \alpha_k = \cos \theta_k a_k + \sin \theta_k b_k \), and \( \beta_k = -\sin \theta_k a_k + \cos \theta_k b_k \), with \( \tan 2\theta_k = (2t'/t') \cos k / \cos 2k \).

The lowest band becomes flat at \(|t'/t| = t/\sqrt{2}\) as shown in Fig. 2. When \(|t'| < t/\sqrt{2}\) there is a single minimum in the lowest band, whereas two minima occur when \(|t'| > t/\sqrt{2}\).

As recently shown [13], for the interacting case the flat band results in a solid phase at lattice filling \( \rho = 1/4 \), but the solid order breaks upon doping due to the proliferation of domain walls. In addition, at \(|t'| = t/\sqrt{2}\) the minimum of \( E_\alpha(k) \) changes from \( k = 0 \) to \( k = \pi/2 \). As a result, for non-interacting bosons, a transition occurs from a superfluid phase at \( k = 0 \) (SF\(_0\)) to a superfluid phase at \( k = \pi/2 \) (SF\(_{\pi/2}\)). Since \( \alpha_{\pi/2} = a_{\pi/2} \), in the SF\(_{\pi/2}\) the B leg is depopulated.

### IV. GROUND-STATE PHASE DIAGRAM

The ground state phase diagram is obtained by means of numerical density matrix renormalization group (DMRG) calculations [21,22]. For our calculation we consider up to \( L = 160 \) sites, with maximally 4 particles per site, and retaining up to 500 states in the density matrix. In order to obtain the signature of possible quantum phase transitions in the system we compute the corresponding order parameters. Particularly relevant is the density structure factor

\[ S(k) = \frac{1}{L^2} \sum_{i,j} e^{ik(i-j)} \langle n_i n_j \rangle, \]

where \( \langle n_i n_j \rangle \) is the density-density correlation between sites \( i \) and \( j \).

In order to quantify the critical point for the SF\(_0\) to Mott-insulator (MI) transition discussed below, we calculate the Luttinger parameter \( K \), which is the power-law exponent of the decay of the single particle correlation function \( \Gamma_r = \langle a_i^\dagger a_j \rangle \). However, in order to obtain the value of \( K \) we evaluate the structure factor \( S(k) \) in the long wave-length limit \( (k \to 0) \), since in this limit [23]

\[ S(k) \propto K |k|/2\pi. \]

We also compute the single particle gap to characterize the gapped MI phase as

\[ E_G = \mu^+ - \mu^-, \]

where \( \mu^+ (\mu^-) \) is the chemical potential for adding (removing) one particle. Finally, the momentum distribution function

\[ N(k) = \frac{1}{L} \sum_{i,j} e^{ik(i-j)} \langle a_i^\dagger a_j \rangle. \]

is particularly interesting as a possible experimental signature of the supersolid phase discussed below.

In the following subsections we discuss the ground-state phase diagram at unit filling, and away from unit filling.
A. Unit filling

Figure 3 shows the ground state phase diagram of model (1) at unit filling, $\rho = 1$. As discussed above, in the non-interacting limit the system exhibits two gapless superfluid phases, SF$_0$ and SF$_{\pi/2}$. In addition to these phases, the system opens as expected a MI phase at small $U$, which at the flat-band point is maintained all the way down to vanishing $U$. The second additional phase is, in contrast, rather unexpected. As we discussed below, this phase is a supersolid (SS), which rather surprisingly occurs at $\rho = 1$ and in the absence of inter-site interactions.

In the following we discuss in detail the different phases for the case $U/t = 3$. In Fig. 4 we plot the thermodynamic limit values of the single-particle gap $\Delta_E$. The MI region is characterized by a finite gap, whereas $E_G \rightarrow 0$ in all other regions. The smooth gap opening at small $|t'|/t$ marks the Berezinski-Kosterlitz-Thouless (BKT) SF$_0$-to-MI transition, characterized by a Luttinger parameter $K = \frac{22}{24}$. By performing a finite size scaling of $K$ computed using Eq. (3), we obtain that the transition for SF$_0$ to MI phase occurs at $|t'|/t \simeq 0.1$ (see Fig. 5(a)). The BKT transition is further confirmed by the scaling of the momentum distribution, $N(k) \propto L^{-1-\frac{23}{24}}$. In Fig. 5(b) we show that the values of $N(k=0)L^{-3/4}$ for different lengths ($L=80$, 120, 160) intersect at the transition point $|t'|/t \simeq 0.1$.

In contrast, the sudden vanishing of $E_G$ for larger $|t'|/t$ at $|t'|/t = 1.4$ in Fig. 4 does not match with a BKT transition. The gapped to gapless transition is, however, confirmed by the single-particle correlation function $\Gamma_r = \langle a_i^\dagger a_{i+r} \rangle$, which decays exponentially in the MI and algebraically for $|t'|/t > 1.4$ (inset of Fig. 4). This transition is likely to be a weak first order transition which could not be confirmed in our numerics.

The superfluid region opening at the large $|t'|/t$ side...
of the MI turns out to be a SS phase. Figure 8 shows the average density \(\text{avg}_{\text{odd,even}}^A\) (\(\text{avg}_{\text{odd,even}}^B\)) at even and odd sites in the A (B) leg. The difference of densities at both legs is not surprising due to the asymmetry between the legs. More interesting is the behavior within a given leg. Whereas for \(\text{avg}_{\text{odd}}^B = \text{avg}_{\text{even}}^B\) for all \(|t'|/t|\), \(\text{avg}_{\text{odd}}^A \neq \text{avg}_{\text{even}}^A\) in the SS region \((1.4 < |t'|/t < 3.1)\) in Fig. 6\) indicating a clear density modulation in this region. The spontaneously broken translational symmetry along the A leg is characterized by the amplitude \(\Delta_n = \text{avg}_{\text{odd}}^A - \text{avg}_{\text{even}}^A\) of the odd-even modulation (inset of Fig. 6\). The broken symmetry translates as well in a difference of bond-kinetic energy \(\Delta_D = \text{avg}_{\text{odd}}^B - \text{avg}_{\text{even}}^B\), where \(\text{avg}_{\text{odd,even}}^D = \frac{1}{L} \sum_{\alpha} (b_{\alpha-1} + b_{\alpha+1} + H.c.)\), which is finite in the SS region (inset of Fig. 6\). The finite \(\Delta_D\) correlates with the V-type dimerization discussed below. The end of the SS region and the onset of the \(SF_{\pi/2}\) phase is marked by the vanishing of both \(\Delta_n\) and \(\Delta_D\), and the depopulation of the B leg.

The SS phase can be further confirmed by a finite peak in \(S(k)\) at non-zero wave vector \(k\). However, we note that the sawtooth lattice breaks a trivial translational symmetry due to which \(S(k)\) shows a peak at \(k = \pm \pi\). Therefore, the presence of the SS phase in the system is revealed by a finite peak in the structure factor at \(k = \pm \pi/2\), confirmed by extrapolation to the thermodynamic limit. In Fig. 7\(\text{top}\) we show, for \(U/t = 3\), the extrapolated value of \(S(k = \pi/2)\), which is finite in the region \(1.4 < |t'|/t < 3.1\), i.e. the SS phase. The extrapolation of \(S(k = \pi/2)\) is shown in detail in Fig. 6\(\text{bottom}\).

### B. Away from unit filling

At this point we consider incommensurate filling. This discussion is particularly relevant, since the presence of an overall harmonic trap, typical of experiments on atoms in optical lattices, results in an inhomogeneous density distribution. In Fig. 5\(\text{we depict our results for } U/t = 2\). In addition to the gapped density-wave phase at \(\rho = 0.25\) at the flat-band point, we obtain gapped phases at \(\rho = n/4\), for all integer \(n \geq 1\) (black lines and squares in Fig. 5\). The gapped phases at these densities are expected to occur at the large interaction limit. The phases at \(\rho = (2n + 1)/4\) with \(n > 1\) are similar to the phase at \(\rho = 1/4\), being comparatively narrow due to small interaction. On the contrary, the gapped phase at \(\rho = 1/2\) is a trivial insulator due to a filled band. Even more relevant is the robustness of the SS phase, which extends over a large parameter region, for densities \(\rho > 0.5\).

We illustrate the behavior of the system for the case of two representative values, \(|t'| = 1/\sqrt{2}\) and \(1.5\) (brown dashed lines in Fig. 8\).

In Fig. 9\(\text{we plot } \rho \text{ as a function of the chemical potential } \mu \text{ for } |t'|/t = 1/\sqrt{2}\). Due to band flatness at that point, at a critical \(\mu\) there exists a macroscopic jump in the density up to \(\rho = 0.25\). This macroscopic jump exists...
for a small region around \( |t'|/t = 1/\sqrt{2} \). This region is marked in the phase diagram by magenta triangles. At \( \rho = 0.25 \) a gap appears marked by a plateau in \( \rho(\mu) \). Then, the system becomes a gapless and compressible superfluid. Further increase in \( \rho \) induces additional gaps as discussed above. In between the gapped plateaus the system is a superfluid.

The dependence of \( \rho(\mu) \) is very different for \( |t'|/t = 1.5 \), since for that value the band is not flat. As a result the system starts at \( \rho \to 0 \) in the SF\( \pi/2 \) phase. In Fig. 9 we observe that the curve \( \rho(\mu) \) is continuous with two kinks at \( \rho \simeq 0.8 \) and 1.2. These kinks correspond to the transition to the SS phase. The abrupt growth of \( \rho \) in the SS phase, shows that the SS phase is highly compressible.

Finally, Fig. 10 shows \( S(k = \pi/2) \) for \( |t'|/t = 1/\sqrt{2} \) and 1.5. For \( |t'|/t = 1.5 \), \( S(k = \pi/2) \) increases in the SS phase, \( 0.8 < \rho < 1.2 \). In contrast, for \( |t'|/t = 1/\sqrt{2} \), \( S(k = \pi/2) \) remains small except at three peaks at \( \rho = 0.25, 0.75 \) and 1.25. The two small peaks at \( \rho = 0.75 \) and 1.25 are due to the presence of two small density-wave phases shown as black squares in Fig. 10. The sharp peak at \( \rho = 0.25 \) corresponds to the density-wave phase reported in Ref. 14.

V. WEAK COUPLING LIMIT

An intuitive insight on the emergence of the SS is obtained from the classical limit of Model [1]. We assume each site to be in a coherent state with a well defined density and phase, 0 or \( \pi \), corresponding to the two possible minima of \( E\alpha(k) \). We consider a simplified model in which \( b_j = \eta \), \( a_{2j} = \xi \), and \( a_{2j+1} = \chi \), such that we allow for both a possible density imbalance between the \( A \) and \( B \) legs, and for an even-odd asymmetry in the \( A \) leg. We may hence minimize the energy, which without loss of generality may be calculated for a four-site unit cell:

\[
(\mathcal{H}) = -4t(\xi\chi + \chi\eta) - 4t'\xi\eta + U(\xi^4 + 2\chi^4 + \eta^4) - \mu(\xi^2 + 2\chi^2 + \eta^2)
\]  

Within this approach the phase diagram splits into three regions (Fig. 11(d)). For \( |t'|/t < 1/\sqrt{2} \) the three coefficients have the same sign, and the particles occupy both \( A \) and \( B \) sites corresponding to the SF\( 0 \)-phase (Fig. 11(a)). For small \( U/t \) and \( |t'|/t > 1/\sqrt{2} \), the \( B \) sites depopulate (\( \eta = 0 \)), the density is homogeneous in the \( A \) sites (\( |\chi| = |\xi| \)), and sign(\( \chi \)) \( \neq \) sign(\( \xi \)), corresponding to the SF\( \pi/2 \) phase (Fig. 11(b)). A sufficiently strong repulsive interaction \( U/t > (U/t)c \) redistributes population to the \( B \) sites. However, how the particles redistribute in the \( A \) leg is crucially determined by the existence of frustrated and un-frustrated plaquettes in the sawtooth lattice. In order to minimize kinetic energy particles favor the un-frustrated V-shaped plaquettes of the

FIG. 9: (Color online) \( \rho(\mu) \) for \( L = 40, U/t = 2, \) and \( |t'|/t = 1/\sqrt{2} \) (blue curve) and 1.5 (red curve).

FIG. 10: (Color online) Structure factor \( S(k = \pi/2) \) for different fillings \( \rho \) for \( L = 40, U/t = 2, \) and \( |t'|/t = 1/\sqrt{2} \) (blue circles) and 1.5 (red squares).

FIG. 11: (Color online) Sketch of the SF\(_0\) (a), SF\(_{\pi/2}\) (b) and SS (c). The circle size is proportional to the local density, whereas \( \pm \) denote the sign. (d) Phase diagram in the weak-coupling limit as function \( U/p \) and \( |t'|/t \) for a fixed (but arbitrary) filling. The SF\(_0\) to the SS phase is shown as a solid line. The dotted and dashed lines depict, respectively, the SF\(_{\pi/2}\)-SS transition line obtained from the variational approach [6] and the roton instability. At \( t = 0 \) SS-order vanishes (thick solid line) resulting in an highly degenerate ground-state, since particles may occupy the uncoupled \( B \) sites in an arbitrary configuration.
sawtooth forming V-shaped dimers. As a result particles break the translational symmetry spontaneously, preferably occupying every second V-plaque (Fig. 11(c)), which leads to a density modulation in the A sites, that characterizes, as mentioned above, the SS phase. Note that this simple picture also predicts a finite $\Delta_D$ in the SS region, as observed in the numerics.

As discussed above, already the classical or weak coupling limit gives an intuitive insight into the formation of the SS phase. We provide in this section some additional details. In Fig. 12 we show typical densities as function of $\mu$, obtained using Model 6. While in the SF$_0$ and SF$_{\pi/2}$ phases the A-sites do not exhibit any density modulation, when entering the SS-phase the average density of the B sites, the solid (black) and dashed (red) lines show densities of odd and even A sites.

**VI. ROTON INSTABILITY.**

Insight on the nature of the SF$_{\pi/2}$-SS transition is obtained in the limit in which $U \ll E_\beta(k) - E_\alpha(k)$ for all $k$. In that case we may project Model 4 onto the lowest energy band:

$$H \approx \sum_k E_\alpha(k) \alpha_k^\dagger \alpha_k + \frac{U}{2} \sum_{q,k,k'} f_{k,k'}^{q,k'} - q \alpha_{k+q}^\dagger \alpha_{k'-q}^\dagger \alpha_{k'+q} \alpha_{k} \alpha_{k},$$

with $f_{k,k'}^{q,k'} = \prod_{l=1}^4 \cos(\theta_{k+l})$. Note that, although the on-site interactions are contact-like, the effective interactions are momentum dependent.

Starting from Eq. 6 and after expanding the interaction part up to second order terms assuming condensation at $q = \pi/2$, i.e. $\alpha_q \approx \sqrt{N} + \alpha_q$ the total Hamiltonian may be written up to constants as $\mathcal{H} \approx \sum_{k>0} A(k) \left( \tilde{\alpha}_k^\dagger \tilde{\alpha}_k + \tilde{\alpha}_{-k}^\dagger \tilde{\alpha}_{-k} + B(k) \left( \tilde{\alpha}_k^\dagger \tilde{\alpha}_{-k} + \tilde{\alpha}_{k} \tilde{\alpha}_{-k} \right) \right)$

This Hamiltonian may be readily diagonalized using a Bogoliubov transformation $\beta_k = \cosh \gamma_k \tilde{\alpha}_k - \sinh \gamma_k \tilde{\alpha}_k^\dagger$, yielding the Bogoliubov spectrum of excitations, $\epsilon(k)^2 = \left( E_A(k) + 2U \rho(1 + \cos 2\theta_k) \right) E_A(k)$ with $E_A(k) = E_A(k) - 2U \rho(1 + \cos 2\theta_k)$. In Fig. 13 we depict the corresponding energy spectrum emerging for finite $\rho U$. As usual the spectrum exhibits a linear (phonon-like) dispersion for $k$ close to $\pi/2$. Interestingly, for finite $\rho U$ it acquires a local minimum at $k = 0$, that resembles the roton dispersion minimum of superfluid He$^{4}$, and that occurs, as for dipolar condensate, due to the momentum dependence of the interactions. For a critical value of $\rho U$ the roton-like minimum reaches zero energy, becoming unstable, marking the transition to the SS. As shown in Fig. 11(d) the critical $\rho U$ for roton instability agrees well with the SF$_{\pi/2}$-SS transition line obtained by the classical model. Hence, we can conclude that the SF$_{\pi/2}$ is destabilized through roton instability that leads to the SS phase.
FIG. 14: (Color online) Momentum distribution $N(k)$ in different regions of the phase diagram shown in Fig. 3 for $U = 3$.

VII. EXPERIMENTAL SIGNATURE

In the section we briefly discuss about the possible signatures of the SS phase in optical lattice experiments using ultracold atoms. The sawtooth lattice can be created by suitably using a superlattice potential on top of the Kagome lattice which has been created recently (see Fig. 16).

In order to obtain the signature of the SS phase we compute the momentum distribution $N(k)$ using Eq. 5. As expected, in $\text{SF}_0$ ($\text{SF}_{\pi/2}$) $N(k)$ has a peak at $k = 0$ ($k = \pi/2$). However, an intriguing feature appears in the SS phase which shows, interestingly, peaks at $k = 0$ and $k = \pi/2$ as shown in Fig. 14. We also plot the peak strengths as a function of $|t'|/t$ at $k = 0$ and $k = \pi/2$ in Fig. 15 which shows the transition from $\text{SF}_0$ - MI - SS - $\text{SF}_{\pi/2}$ for $U = 3$ and $\rho = 1$. Hence, the appearance of the SS phase may be directly monitored in time-of-flight experiments from the multi-peaked momentum distribution.

VIII. CONCLUSIONS

We have discussed a novel mechanism for the formation of lattice supersolids for the particular case of a sawtooth lattice. The mechanism is based on the selective population of un-frustrated plaquettes in the presence of frustrated and unfrustrated plaquettes, and hence we expect supersolids in other lattices fulfilling that property. We have shown that the supersolid exists for a broad range of lattice fillings, including various commensurate fillings, in particular unit filling. Interestingly the supersolid may be revealed not only by in-situ measurements, but by monitoring the momentum distribution in time-of-flight measurements. Since frustrated lattices, in particular sawtooth, may be realized using state of the art techniques, our results open hence a new feasible path for realizing supersolids in existing experiments with ultra cold atoms in optical lattices, without the need of long-range interactions.

Acknowledgments

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The sawtooth chain considered has even number of sites so that we have an extra site in the end of the lattice. This assumption enables us to get rid of any possible degenerate dimerized phase which may possibly occur in the large $U$ limit (see O. Derzhko, J. Richter, M. Maksymenko, Int. J. Mod. Phys. B 12, 1530007 (2015)).

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