Report on "Systematic Analysis of Crystalline Phases in Bosonic Lattice Models with Algebraically Decaying Density-Density Interactions"

In the present manuscript, Koziol *et al.* propose an efficient algorithm to find the classical ground states of different experimentally relevant long-ranged interacting Hamiltonians. Their central idea is to identify the most energetically favorable diagonal order in the space of all possible unit cells and employ a resummation technique to encapsulate the effects of all the long-ranged tails within this unit cell.

The work itself is theoretically sound and the manuscript is also well-written and straightforward to follow. I personally believe that these results, even though classical, would be extremely useful to the ultracold-atoms community because the solid density-wave-ordered states may be regarded as starting points both to benchmark experiments and to incorporate quantum corrections. Moreover, there are often subtle effects from the long-ranged dipolar ($1/r^3$) or van der Waals ($1/r^6$) interactions—which are hard to quantify in simple mean-field calculations—and the careful analysis outlined in this paper bridges this gap. Therefore, I would recommend its publication in *SciPost Physics* after some revisions (listed below).

However, I do have a few other questions and comments that I would appreciate being addressed in a revised version of the manuscript first:

a. In Eqs. (3)–(5), I believe the left-hand sides should read as $\mathcal{L}(\boldsymbol{t}_1, \boldsymbol{t}_2, \ldots)$, not $\mathcal{L}(\boldsymbol{t}_1, \boldsymbol{t}_1, \ldots)$.

b. In Sec. 3.1, could the authors provide some analytical estimates for the extent (width in V/U) of the different orders as a function of the spacing between defect lines d_s? In the same vein, if possible, some back-of-the-envelope calculations of the extents of the different solid orders in Table 2 would be useful.

c. On page 12, the authors refer to the "$1, 2$-Phase" or the "$3, 4$-Phase" but this notation has not been introduced earlier. I understand that this is referring to the possible number of bosons on different sites within that phase but for the sake of precision, this should be defined.

d. In Eq. (19), suppose we add a chemical potential μ, which we then vary instead of V/U. In this case, the phase diagram should host a devil's staircase as predicted by Burnell *et al.*, *Phys. Rev. B* 80, 174519 (2009). Could the authors demonstrate that their methodology is able to obtain this devil's staircase (of course, subject to the availability of rational filling fractions dependent on the maximum size chosen for the unit cell)? This would be an important result that should strengthen the paper.

e. In Fig. 9, for the sake of consistency with Fig. 11, could the authors please arrange the different ordered states in increasing order of the filling fraction f? I understand that the current arrangement was chosen to demonstrate the particle-hole symmetry but jumping back and forth between different filling fractions is confusing.

f. On page 24, the authors write that "*The dimer covering, which we find to have the lowest energy at* $\Omega = 0$*, is depicted in Fig.* 11 *and has a dimer alignment without any resonating plaquettes.*" This state disagrees with the 72-site pinwheel VBS found in Ref. 97, presumably due to the truncation of the interactions in the latter. It would be helpful if the authors could plot the VBS obtained as a function of n, where one retains up to n-th neighboring interactions. This is of great experimental relevance because the small energy scales of the interaction tails might not be resolvable on the dynamical time scales of the experiments.

g. Lastly, one of the attractive features of this paper is its immediate utility to practitioners in the field of ultracold atomic physics and quantum magnetism. Therefore, in order to maximize the benefits to the physics community at large, I would strongly urge the authors to consider making their algorithm publicly accessible, perhaps as a Github package, so that people can use the methods developed in this work for their individual Hamiltonians of interest.