Reviewers' comments:

Reviewer #2 (Remarks to the Author):

The manuscript "How creating one additional well can generate Bose-Einstein condensation" investigates interacting bosons in a quasi-one-dimensional ring lattice that may be globally coupled via a site in the center of the ring.
The manuscript's finding is that the global coupling of all sites on the ring has a strong effect on the degree of condensation of the system.
The manuscript lacks some clarity and discussion/contrast with other results in the field that analyze the degree of condensation. In particular, the topic of the presence or absence of fragmentation is not touched upon. I would like to invite the authors to revise their manuscript using my following questions to guide them:

1) The introduction points out that there are predominantly mean-field approaches applied to Bose-Einstein condensation (BEC). There's also a wealth of work on beyond-mean-field physics of BEC, that should be at least mentioned. For instance, using methods like MLMCTDHB and MCTDHB (Phys. Rev. A 77, 033613 (2008), J. Chem. Phys. 139, 134103 (2013), Rev. Mod. Phys. 92, 011001 (2020)), DMRG, and exact diagonalization approaches. For a balanced introduction to the subject, these approaches and their results on BEC (for instance, Phys. Rev. Lett. 103, 220601 (2009), Phys. Rev. A 89, 023602 (2014)) could be discussed and the results of the present manuscript could be contrasted against those findings.

2) The sentences following "To be more specific... faced while realizing BEC" are very vague an not helpful as the key players "topology", "control parameter",... remain undefined. I invite the authors to rewrite this paragraph and get it to the point by introducing the specific system that they study. As a suggestion: use the sentences that were written to describe Fig. 1, "As it is illustrated in Fig.~1...", and rephrase them accordingly.

3) Carefully revisit some of the text regarding point 1), for instance "common theoretical studies ... weakly interacting bosons." There are plenty of counter examples of works that study beyond-mean-field physics and the effects of interactions.

4) "ratio between kinetic and interaction energy": What about the potential energy/on-site energy offset? At least say that you do consider it to be absent?

5) Would it make sense to cite (Phys. Rev. Lett. 81, 3108 (1998), Nature 415, 39 (2002)) as a reference for the Bose-Hubbard model?

6) Somewhere following the Hamiltonian, I would invite the authors to discuss the limitations of the Hubbard description: here is some literature that demonstrates its breakdown (Phys. Rev. Lett. 103, 220601 (2009), New J. Phys. 13 043003 (2011), J. Phys. B: At. Mol. Opt. Phys. 47 225303 (2014), Phys. Rev. A 91, 033611 (2015), Phys. Rev. A 95, 013625 (2017)) also for long-range interactions (New J. Phys. 21 053044 (2019), Phys. Rev. Lett. 125, 093602 (2020)).

7) The explanation on s/t, "Hence, changing..." could help make the introduction clearer.

8) "qualitatively exact" should be rephrased or at leased explained, as something is either "qualitative" or "exact".

9) Fig. 2 is hard to decipher. Enlarging or rearranging it might help. Also, the meaning of the symbols (crosses, circles) could be explained in the caption and not only in the text.

10) Fig. 4 is hard to understand, as the vertical axis is in absolute particle numbers. It would be helpful to plot the number of condensed bosons as a fraction of the total number of particles.

Moreover, it would be instructive to give the particle numbers investigated in Fig. 4a) as labels.

11) Is there fragmentation, i.e., several macroscopic eigenvalues of the one-body density matrix, in some of the investigated cases? I invite the authors to show a plot of the other eigenvalues of the one-body density matrix.

12) At what sites is the condensation criterion broken/maintained? I invite the authors to compute the Glauber correlation functions of first and second order to get a spatial understanding of the nature of BEC in their system (cf., for instance, Phys. Rev. A 78, 023615 (2008)). These quantities are straightforwardly available to the authors as they have also computed "one-[...]site and two-[...]site reduced density matrices".

Reviewer #3 (Remarks to the Author):

Bose condensation in low dimensions has always been an interesting and intriguing topic from a quantum point of view. The role of interactions, in this case, is of great relevance, not just changing parameters, but changing the nature of the phenomena. In this work, the authors demonstrate a spatial configuration of potential in practically 1D, in the form of an array of potentials in the form of a ring. The addition of a central well allows overcoming problems associated with strong interactions in the formation of the BEC.

In this sense, the system, now practically 2D, is interesting, new, and could allow a series of relevant investigations, difficulties to be idealized with the traditional confinement configurations.

This fact, by itself, is already interesting and may open up possibilities. The manuscript is well presented, clear written and all of this together already guarantees that it can be recommended for publication. It remains to be discussed whether there is a need for a Communication type publication. In this sense, I think it's on the board line, but I don't think it's far in the quality and relevance of the articles published in this journal. I suggest acceptance of the referred manuscript.

As a suggestion for the authors, there are many references discussing the modification of the nature of transitions in low dimension due to the interaction. A survey on that could be carried out and old references included

Reply to the Referees

December 15, 2020

We thank the referees for their effort and their comments to which we provide point-by-point replies below.

Referee #3 :

We are glad to read that this referee states that our contribution *"is interesting, new, and could allow a series of relevant investigations"* and also remarks *"The manuscript is well presented, clear written ..."*. Concerning her/his suggestion to add *"references discussing the modification of the nature of transitions in low dimension due to the interaction"* we have added Refs.[19-22]. References [78-83] discussing that point were already cited in the original manuscript.

Referee #2 :

We gratefully acknowledge the critical comments on our manuscript. This criticism does not concern the soundness and quality of our results, but parts of the manuscript's presentation. Several of her/his comments have led us to improve the presentation.

In addition, the present referee lists 14 articles which she/he suggests(?) to be cited. Twelve of them(from the research group of Prof. L. S. Cederbaum or of his former coworkers, Prof. O. E. Alon, Dr. A. U .J. Lode, Prof. P. Schmelcher, have in common that two methods(MCTDHB and MLMCTDHB) to rewrite the time-dependent Schrödinger equation are used. "TD" in those acronyms stands for **time-dependent**. Nine of these papers study time-dependent phenomena of Bose-Einstein condensates(BEC). Since this is a rather different subject than the one of our work on ground state investigation, we feel that citing those nice publications in our context would be less appropriate.

Now we will discuss the various points:

1) The introduction points out that there are predominantly mean-field approaches applied to Bose-Einstein condensation (BEC). There's also a wealth of work on beyond-mean-field physics of BEC, that should be at least mentioned. For instance, using methods like MLMCTDHB and MCTDHB (Phys. Rev. A 77, 033613 (2008), J. Chem. Phys. 139, 134103 (2013), Rev. Mod. Phys. 92, 011001 (2020)), DMRG, and exact diagonalization approaches. For a balanced introduction to the subject, these approaches and their results on BEC (for instance, Phys. Rev. Lett. 103, 220601 (2009), Phys. Rev. A 89, 023602 (2014)) could be discussed and the results of the present manuscript could be contrasted against those findings.

Our "Introduction" mentions not only the mean-field theory(Gross-Pitaevskii equation) but also perturbational approaches like the seminal work by Bogoliubov. Both methods mentioned by the referee represent one of many quite different methods. A *"balanced introduction"*(what this referee is requesting) would require to cite and to discuss many of those methods like DMRG(which is applied in our work), exact diagonalization, Quantum-Monte-Carlo, MLMCT-

DHB, MCTDHB, density functional theory, density matrix functional theory, slave-boson approach, renormalization theory, etc.). This does not make much sense, however, since our contribution is a short Communication rather than a Review. Yet, in order to clarify this point we have added new text at the end of the 1st paragraph on page 1:

Although these two widely used approaches have led to a deeper understanding of BEC, their range of validity is limited. To go beyond that limitation, various methods were developed(see e.g. Refs.[19-22]).

We also added new Refs.[1-4] at the very beginning of our manuscript(2nd line)

Since the scientific focus of the five papers mentioned by the referee is on time-dependent phenomenon which differs completely from our study of the time-independent ground state properties it would not make that much sense to contrast the results of those papers with ours.

2) The sentences following "To be more specific... faced while realizing BEC" are very vague an not helpful as the key players "topology", "control parameter",... remain undefined. I invite the authors to rewrite this paragraph and get it to the point by introducing the specific system that they study. As a suggestion: use the sentences that were written to describe Fig. 1, "As it is illustrated in Fig. 1...", and rephrase them accordingly

Although the term *control parameter* is often used in Physics we removed "control". It describes a parameter which can be varied experimentally, i.e. it can be controlled. We agree that the part of the text where *topology* was mentioned is vague . We tried to improve the corresponding parts:

... by changing just a single parameter, s/t, which is the ratio of the model's two hopping rates s and t, as explained below. Remarkably, as we will show, this establishes a new mechanism which effectively increases the mobility of the bosons.

The next sentence in this paragraph is not vague. It states the well-known fact that a BEC phase may occur if the kinetic energy effects become more dominant when those from the pair interactions. This also holds for its last sentence stating that the existence of a gap in the excitation spectrum is sufficient to make a BE-condensate robust under thermal or quantum fluctuations.

3) Carefully revisit some of the text regarding point 1), for instance "common theoretical studies ... weakly interacting bosons." There are plenty of counter examples of works that study beyond-mean-field physics and the effects of interactions.

We removed that last sentence of that paragraph

4) "ratio between kinetic and interaction energy": What about the potential energy/on-site energy offset? At least say that you do consider it to be absent?

This remark is correct. To clarify this point we have added in the 4th. line of subsection “Model Hamiltonian” the following sentence:

In case of systems which are inhomogeneous, e.g., due to the presence of an external field or disorder, the occurrence of BEC will also depend on these quantities.

5) Would it make sense to cite (Phys. Rev. Lett. 81, 3108 (1998), Nature 415, 39 (2002)) as a reference for the Bose-Hubbard model?

It makes sense to cite the Letter by Jaksch et al., which we did(new Ref.[47]). Since our hard-core boson-model does not exhibit a transition from a superfluid to an insulating phase and the crossover from quasi- to maximum condensation does not have anything in common with the superfluid-insulator transition the citation of the famous article by Greiner et al. does not seem to be necessary. In the 2nd. line below Eq. (1) we added :

It was shown that the Bose-Hubbard model can be experimentally realized by ultra-cold bosonic atoms in an optical lattice [47].

6) Somewhere following the Hamiltonian, I would invite the authors to discuss the limitations of the Hubbard description: here is some literature that demonstrates its breakdown (Phys. Rev. Lett. 103, 220601 (2009), New J. Phys. 13 043003 (2011), J. Phys. B: At. Mol. Opt. Phys. 47 225303 (2014), Phys. Rev. A 91, 033611 (2015), Phys. Rev. A 95, 013625 (2017)) also for long-range interactions (New J. Phys. 21 053044 (2019), Phys. Rev. Lett. 125, 093602 (2020)).

We do not doubt that there are limitations of the *one-band* Bose-Hubbard model. But, on the other hand it was demonstrated by an extremely large number of investigations over three decades that this model is capable to successfully describe numerous physical phenomenon for bosonic systems which are consistent with experimental findings. The crossover between quasi-condensation and the maximum possible condensation studied by us is not an artefact of the lattice character of our model. As also argued in the section “Potential experimental realization” this crossover, as well, will occur for interacting bosons in an appropriately chosen two-dimensional trap potential shown in Fig. 6. Since our focus is on the *qualitative* change from quasi- to maximum condensation *quantitative* differences, e.g., for the condensate number obtained from our lattice model and a continuum model is less relevant.

To be more specific we note that the DMRG result in Fig. 4a for our lattice model and $\log(\tilde{s}) = -3$ fits perfectly the result from the continuum model of impenetrable bosons(Lieb-Liniger model with infinite coupling strength) for all five values of d. This is pointed out in our original manuscript. Looking now to Fig. 4b **just the opposite of the referee's warning happens**. For higher densities the numerically exact result at $\log(\tilde{s}) = -3$ is not in agreement with that from the continuum model(dashed lines). This means that the continuum model can not describe all features of the lattice model. This also was pointed out in our original manuscript.

Therefore, concerning the goal of our contribution there is no need to discuss the limitations of the Bose-Hubbard model. This also holds for both references on long range interactions by B. Chatterjee et al. PRL 125, 093602 (2020)). The second paper(S. Dutta et al. New J. Phys. 21 053044 (2019)) uses a contact potential, which is the opposite of a long range potential. We also do not quite understand why this referee mentions long range *interactions*. Our model has no long range interactions, but long range *hopping*.

7) The explanation on s/t, "Hence, changing..." could help make the introduction clearer.

This is correct and has been done(see the bold text in point 2)

8) "qualitatively exact" should be rephrased or at leased explained, as something is either "qualitative" or "exact".

The Referee is right. Of course, we wanted to say "qualitatively correct". We changed the text five lines below Eq. (3) as follows:

... important qualitatively correct features of the spectrum...

9) Fig. 2 is hard to decipher. Enlarging or rearranging it might help. Also, the meaning of the symbols (crosses, circles) could be explained in the caption and not only in the text.

We have enlarged the height of that figure and increased some of the level spacings. We also explained the meaning of the symbols in the caption

10) Fig. 4 is hard to understand, as the vertical axis is in absolute particle numbers. It would be helpful to plot the number of condensed bosons as a fraction of the total number of particles. Moreover, it would be instructive to give the particle numbers investigated in Fig. 4a) as labels.

Yes, it is more convenient to add N as labels, which we did.

The reason why we did not scale N_0 by the total particle number N is threefold: (i) Since N is still small and not yet macroscopic the use of the "absolute" scale seemed to use not inappropriate (ii) more important, on the left and right, i.e. for $\log(\tilde{s}) < -2$ and $\log(\tilde{s}) > 2$, respectively, the plateaus would become more close. In that case one of our main messages would not become clearly visible This is the finding that the DMRG-results in Fig. 4a (low density) become almost identical to the results of the continuum model of impenetrable bosons(dotted lines) for very small $\tilde{s}$, whereas in Fig. 4b(finite densities) they are different. Independent on the density n, Fig. 4a and 4b illustrate that the large-$\tilde{s}$ behavior of the DMRG-results are well described by the corresponding result from our effective Hamiltonian(the horizontal lines). This illustration, as well, would be much less clearly visible, if we would have used the scaling. (iii) There is a tiny "small particle number"-effect shown by the solid lines in Fig. 4a. It is discussed in the original text that N_0 as function of $\tilde{s}$ is slightly non-monotone close to $\tilde{s} = 1$. This effect is most pronounced for $N = 2$. Since this effect is already not easily visible it would become even less visible under scaling, and we did not want to enlarge that figure even more.

11) Is there fragmentation, i.e., several macroscopic eigenvalues of the one-body density matrix, in some of the investigated cases? I invite the authors to show a plot of the other eigenvalues of the one-body density matrix.

For $s/t \to 0$ and $s/t \to \infty$ the answer is no. For s/t small enough there is only quasi-condensation. Hence there is even no eigenvalue of the one-body reduced density matrix(1-RDM) of order N. For s/t large enough the ground state of our model is given by the ground state of the effective Hamiltonian derived in the Supplementary Information. This ground state is known analytically(see manuscript). From this it is straightforward to calculate analytically all eigenvalues of the corresponding 1-RDM: The largest one is given by $N_0(N, n) \simeq N(1-n)$ and all the other eigenvalues are degenerate, $N_k(N, n) \simeq n^2$ for $k = 1, 2, ...d-1$, i.e., no further eigenvalue exists besides N_0 which is macroscopic in N. Consequently, no fragmentation exists. Because s/t interpolates between natural occupation numbers of order $\sqrt{N}$ for $s/t = 0$ and a *single* occupation number of order N it is very unlikely that fragmentation could occur in between for any finite s/t.

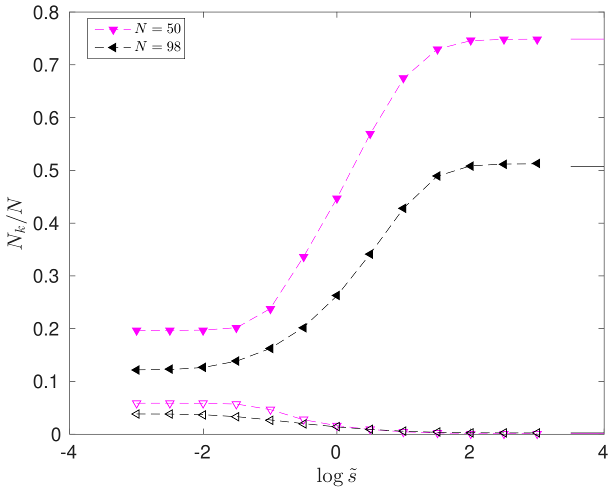

Figure 1: DMRG result for the two largest natural occupation numbers scaled by the total number N of particles as a function of $\log(\tilde{s})$ for $d = 199$ and $N = 50, 98$. The full symbols refer to N_0 and the open ones to N_1

The figure above presents the DMRG-result for the two largest eigenvalues N_0/N and N_1/N scaled by N for $d = 199$, $N = 50$ and $N = 98$. It supports the conclusion that there is no fragmented condensation. For $\log(\tilde{s}) < -1$ both eigenvalues are of similar size. But this does not mean fragmentation because both eigenvalues are of order $\sqrt{N}$ and not of order N. Since there is no fragmented condensation in our model, and more important, it has not been our motivation to study such a phenomenon, we have not added that figure.

But we have added a new paragraph in the section "Potential experimental realization"(see 2nd last paragraph):

If the trap potential in Fig. 6 is chosen such that it represents a good experimental realization of the 'wheel' lattice (cf. Fig. 1) there is true condensation for sufficiently large s/t. In particular, since only a single one-particle state (zero-momentum state) is macroscopically occupied, no fragmented condensation exists per definition. This is consistent with the expectation that homogeneous bosonic systems with purely repelling pair interactions do not exhibit fragmented condensation [4]. Although the presence of the central well(central site) makes the system inhomogeneous it can not generate fragmentation, because it accommodates maximally one HCB, only. But increasing the width of the central well on the right of Fig. 6 such that this well can accommodate a "macroscopic number of bosons of an ultracold gas, a situation similar to the double-well-like trap potential in one dimension occurs [78]. As shown in that reference, fragmented condensation may then occur if the barrier height of the double well is high enough.

12) At what sites is the condensation criterion broken/maintained? I invite the authors to compute the Glauber correlation functions of first and second order to get a spatial understanding of the nature of BEC in their system (cf., for instance, Phys. Rev. A 78, 023615 (2008)). These quantities are straightforwardly available to the authors as they have also computed "one-[...]site and two-[...]site reduced density matrices".

The last paragraph of section ""Spectral properties, BEC and entanglement" describes qualitatively how the correlations between two ring sites and between a ring and the central site behave under variation of s/t. As stressed in that paragraph these findings, based on using the mutual information, are completely consistent with the physical behavior related to the crossover from a quasi-condensate to maximum true condensation. For instance, in the regime of quasi-condensation an algebraic decay of the mutual information is found as it was proven for the decay of the off-diagonal part of the one-body matrix(Ref.[34]). In case of true condensation the off-diagonal part exhibits long-range correlations. Since our manuscript is written as a "Communication" and not as an extended research article, we do not think that inclusion of such additional quantities is necessary.

Conclusion We have revised our manuscript on the basis of the referees' comments. We included also several new references as described above(see also "List of changes").

List of changes:

1. end of the first paragraph on page 1:
   we inserted: **Although these two widely used approaches have led to a deeper understanding of BEC, their range of validity is limited. To go beyond that limitation, various methods were developed(see, e.g., Refs. [19-22]).**
   We also added new Refs.[1-4] at the very beginning of our manuscript(2nd line)

2. last paragraph on page 1:
   we deleted: **deforms the underlying topology to** and deleted the last sentence: **Accordingly, our work overcomes the undesirable restriction of common theoretical studies in the field of ultracold gases to ideal or weakly interacting bosons.**

3. In the 4th line of section "Model Hamiltonian" we inserted:
   In case of systems which are inhomogeneous, e.g., due to the presence of an external field or disorder, the occurrence of BEC will also depend on these quantities.

4. 2nd line below Eq. (1):
   new text and reference was inserted:
   It was shown that the Bose-Hubbard model can be experimentally realized by ultra-cold bosonic atoms in an optical lattice [47].

5. five lines below Eq. (3): we inserted:
   ... important qualitatively correct features of the spectrum...

6. Figure 2:
   We have enlarged the height of that figure and increased some of the level spacings. We also explained the meaning of the symbols in the caption

7. Fig 4a:
   we added the particle number as labels

8. fragmentation
   we added a new paragraph in the section "Potential experimental realization":
   If the trap potential in Fig. 6 is chosen such that it represents a good experimental realization of the 'wheel' lattice (cf. Fig. 1)

there is true condensation for sufficiently large s/t. In particular, since only a single one-particle state (zero-momentum state) is macroscopically occupied, no fragmented condensation exists per definition. This is consistent with the expectation that homogeneous bosonic systems with purely repelling pair interactions do not exhibit fragmented condensation [4]. Although the presence of the central well(central site) makes the system inhomogeneous it can not generate fragmentation, because it accommodates maximally one HCB, only. But increasing the width of the central well on the right of Fig. 6 such that this well can accommodate a "macroscopic number of bosons of an ultracold gas, a situation similar to the double-well-like trap potential in one dimension occurs [78]. As shown in that reference, fragmented condensation may then occur if the barrier height of the double well is high enough.

REVIEWERS' COMMENTS:

Reviewer #4 (Remarks to the Author):

The authors study dimensional effect in condensation by considering a ring-shaped tight-binding model that is continuously transformed into a star-shaped system with an effective “infinite-range” hopping. The manuscript provides a nice DMRG calculations and analysis of the system where quantum effects of interactions have been included.

I tend to share the reservations of Reviewer 3 whether the work, however, warrants publication in Communications Physics. I have in particular difficulties identifying what are the important results for the research community that one learns from the numerics and the neat model.

Furthermore, while I believe that the authors have provided a comprehensive list of references, I agree with Reviewer 2 that the first part of the introduction could be better. At least to my taste, the first 1.5 paragraphs are too general and tell less about the reasons why this specific work is important and why readers should be interested. This is also relevant regarding my reservations in the previous paragraph.

I believe the work would consequently be more suitable as a research article than as a Communication.

Reply to the Referee

January 11, 2021

We thank this Reviewer for her/his effort and comments.

The Reviewer rises two points. One concerns the *"identification what are the important results"* and second that *"the first part of the introduction could be better ... at least to my taste , the first 1.5 paragraphs are too general and tell less about the reasons why this specific work is important and why readers should be interested."*

We agree that the first two paragraphs are rather general and do not explain why our results are important. However, the first of these paragraphs intend to introduce Bose-Einstein condensation(BEC) on a rather general level and the second one describes the phenomenon of quasi-condensation. This should serve as an introduction for a the broader readership of Communication Physics. Yet, to take into account the referee's comment we have eliminated the following lines from the first paragraph:

"From an experimental point of view, this has been a remarkable achievement. Interacting bosons had to be trapped and cooled down to extremely low temperatures and a sufficiently small particle density was required to reach the regime of effectively weak interactions." and have inserted a few lines below **"(corresponding to the experimental situation for ultracold gases)"**

The importance of our results was described, however, in the third paragraph of the Introduction, in the section "Model Hamiltonian" below Figure 1 and more comprehensively in the section "Discussions". To comment more on the relevance of our work, we have split the original third paragraph of the Introduction into three new ones in order to relate our work to already existing investigations(the new third and fourth paragraph) and to explain better why our model is original and our results are of importance(new fifth paragraph). This fifth paragraph also contains two new references, [46] and [48]. Here are three examples(taken from the fifth paragraph) pointing out the originality and importance of our work:

"It is the challenge of the present work to propose and investigate a lattice model for strongly interacting bosons which allows one to drive such a transition by changing just a single parameter."

"One of our major results is to establish by this model a mechanism which can generate 'infinite' range hopping by increasing s/t. This is important since enhancing the boson's mobility allows to overcompensate the destructive effects of the repulsive interactions, leading finally to maximal possible condensation, despite infinitely strong repulsion"

"The other important result concerns the application of tools from quantum information theory. We show that the mutual information possesses the qualitatively similar dependence on s/t as the number $N_0(N)$ of condensed bosons. This supports the connection between

the behavior of an order parameter and of entanglement at a quantum phase transition even for the transition(or crossover) from a quasi-condensate to a true one."

Finally, the Reviewer considers our DMRG results as *"nice"*. But she/he does not make any comment on one of our key achievements, i.e., the new kind of analytical approach which allowed us to prove, e.g., the existence of an excitation gap. Therefore, we added new text in the first paragraph of the section "Discussion"

"Without solving the model's eigenvalue equation exactly, our analytical approach(see the section on "Spectral properties" and in particular the Supplementary Methods) allows us to show on a qualitative level why an excitation gap occurs in the N-particle spectrum, which usually is highly demanding. Similarly to, e.g. superconductivity, the quantum Hall effect and the Haldane phase the existence of such a gap has an enormous influence on the physical behavior, e.g., making the BE-condensate robust to thermal noise and perturbations in general"