Condensation driven by a quantum phase transition

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Abstract

The grand canonical thermodynamics of a bosonic system is studied in order to identify the footprint of its own high-density quantum phase transition. The phases displayed by the system at zero temperature establish recognizable patterns at finite temperature that emerged in the proximity of the boundary of the equilibrium diagram. The gapped phase underlines a state of collectivism/condensation at finite temperature in which particles coalesce into the ground state in spite of interacting attractively. The work establishes a framework that allows to study the phenomenon of condensation under the effect of attraction.

Keywords: phase transitions, boson systems, condensation

1. Introduction

The understanding of collectivism is a crucial task in the search for practical applications where a number of phases taking place in the low-energy range could be utilized in mass-produced technology. The process by which a large number of particles, in particular bosons, collectively occupy the same single-body state gives rise to coherent phases where the features of a single state magnify and therefore manifest at the macroscopic level. The archetype of collectivism is Bose–Einstein condensation [1], a mechanism that constitutes the interpretative ground of other phenomena like superfluidity or superconductivity. In essence, condensation is driven by statistical effects at the single-body level, but interaction cannot be completely suppressed in any practical scenario. The role of attractive interaction, in particular, has proved detrimental in a number of studies [2–12], but experimental evidence of condensation in attractive systems has been reported [13]. In this context there must be a range over which collectivism can be

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sustained under the effect of interaction, especially when the interaction role can be captured using single-body terms. The relevance of this phenomenon is notorious in times when the first prototypes of quantum computation have demonstrated quantum supremacy \([14, 15]\) and control mechanisms are increasingly necessary to extent the current capabilities \([16]\). This has boosted the interest in the realization of novel collective phases such as the molecular condensate \([17, 18]\), which in turn evidences the need of a better understanding of the process of condensation under attractive fields since it may prove a precursor of molecular formation.

Let us consider a system of one-species bosons that can tunnel between two equal-energy wells \([19]\). Bosons can interact among them only when they occupy the same well. This interaction is attractive, so it tends to pack bosons together. The system is modeled via the next quantized Hamiltonian

\[
\hat{H}_M = \delta (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) - i\gamma (\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1) - \frac{\lambda}{M} (\hat{m}_1^2 + \hat{m}_2^2).
\] (1)

Ladder operators obey standard bosonic commutation rules, \([\hat{a}_1, \hat{a}_1^\dagger] = [\hat{a}_2, \hat{a}_2^\dagger] = 1, [\hat{a}_1, \hat{a}_2] = 0\). The number operators

\[
\hat{m}_1 = \hat{a}_1^\dagger \hat{a}_1, \quad \hat{m}_2 = \hat{a}_2^\dagger \hat{a}_2, \tag{2}
\]

determine the particle occupation at each well. Integer \(M\) is the total number of particles in the space of \(\hat{H}_M\), so that \(M = \hat{m}_1 + \hat{m}_2\). Constants \(\gamma\) and \(\lambda\) modulate the intensity of hopping and interaction respectively. Both are considered strictly positive in this work. Constant \(\delta\) modulates the intensity of a hopping process in which the phase of one well with respect to the other is unchanged. From here on the energy scale is chosen so that \(\delta = 1\). This choice automatically determines the unit of energy and renders the other variables dimensionless. By definition \(\hat{H}_0 = 0\). Hamiltonian (1) has the essential elements of a Bose–Hubbard model, which has been studied from the perspective of the grand-canonical formalism as a descriptor of the transition between Mott insulator and superfluid \([20]\) and also verified experimentally with ultracold atoms \([21]\). Hopping terms with complex coefficients have been justified in a number of contributions \([22, 23]\). Another feature of the proposed Hamiltonian is that interaction is attractive and has been scaled with respect to the number of particles. Such a feature can also be seen in related models such as the Lipkin–Meshkov–Glick model and the infinite-range Ising model, from which Hamiltonian (1) can be obtained as a second quantization \([24]\). From the perspective of quantum field theory Hamiltonian (1) represents a zero-dimensional model in the sense that operators do not depend on continuous variables.

Assuming that the ground state adopts a collective form, it can be written as

\[
|G(\theta, \varphi)\rangle = \frac{\hat{b}_1^M (0, 0)}{\sqrt{M!}}, \quad \hat{b}_1^\dagger = \hat{a}_1^\dagger \cos \theta - \hat{a}_2^\dagger e^{i\varphi} \sin \theta, \tag{3}
\]

so that \([\hat{b}_1, \hat{b}_1^\dagger] = 1\). The angle domains are \(0 \leq \theta \leq \pi/2\) and \(0 \leq \varphi < 2\pi\), ensuring that different angle pairs correspond to genuinely different modes. In order to find the correct angles, the energy function

\[
E(\theta, \varphi) = \langle G(\theta, \varphi) | \hat{H}_M | G(\theta, \varphi) \rangle, \tag{4}
\]
is minimized over $\theta$ and $\varphi$. From the procedure shown in appendix A it follows that to first (highest) order in $M$ the system displays two distinct phases determined by the value of $\lambda$ relative to the critical value

$$\lambda_c = \sqrt{1 + \gamma^2}. \quad (5)$$

In the region $\lambda \leq \lambda_c$ the energy displays a single minimum localized at

$$\theta^* = \frac{\pi}{4}, \quad \cos \varphi^* = \frac{1}{\lambda_c}, \quad \sin \varphi^* = \frac{\gamma}{\lambda_c}. \quad (6)$$

The corresponding ground state energy is

$$E_{\lambda \leq \lambda_c}^* = -M \left( \frac{\lambda_c + \lambda}{2} \right). \quad (7)$$

From quantum theory it is known that because in this phase the ground state is non-degenerate it must display the Hamiltonian’s symmetries. Hamiltonian (1) commutes with the antiunitary operator composed by the swapping of subscripts $1 \leftrightarrow 2$ followed by complex conjugation. As a consequence, the number of particles on each well must be the same.

In the region $\lambda \geq \lambda_c$ the energy displays two equal minima located at $(\theta_1^*, \varphi^*)$ and $(\theta_2^*, \varphi^*)$. Here $\varphi^*$ is the same than in equation (6). In addition

$$\theta_1^* = \frac{1}{2} \arcsin \frac{\lambda_c}{\lambda}, \quad \theta_2^* = \frac{\pi}{2} - \theta_1^*. \quad (8)$$

Notice that by making $\theta$ different from $\pi/4$ the balance of occupation between the wells is broken and the proposed solutions do not independently display the Hamiltonian’s inversion symmetry. The corresponding ground state energy is

$$E_{\lambda \geq \lambda_c}^* = -M \left( \lambda + \frac{\lambda_c^2}{2\lambda} \right). \quad (9)$$

The phase change is rooted in a change in the Hamiltonian spectrum, which goes from non-degenerate for $\lambda < \lambda_c$ to two-fold degenerate for $\lambda \geq \lambda_c$. In the latter case the equilibrium configuration corresponds to a maximally mixed state in the space spanned by two linearly independent ground states. However, it is often argued that small perturbations spontaneously tip the scale to either of the constituent pure-states, such that the phase change is equivalent to a continuous break of symmetry of a pure ground-state as a function of the Hamiltonian’s parameters. This process is known as a second order quantum phase transition and takes place at zero temperature since it is in this instance that the equilibrium state coincides with the ground state. Here it is intended to show that under specific conditions this quantum phase transition can manifest at finite temperature, although not as a symmetry breaking of a quantum state in pure form but as a change in the collective behavior of a grand canonical ensemble of particles.

2. Thermodynamic state of the open system

When the system is embedded in a bath of inverse temperature $\beta$ and chemical potential $\mu$ it eventually reaches thermodynamic equilibrium. This equilibrium state is represented by a
Figure 1. Left. Colored regions represent the parameter zones where the grand partition function converged (equilibrium zones). Right. Relative mean number of particles in the mode perpendicular to the mode with maximum occupation, as defined by equation (22). Perpendicular occupation falls when approaching the divergence from inside the case-1 region or through the boundary separating the cases, showing that to first order the particles tend to gather all in the mode with maximum occupation. This mode coincides with the ground state mode in the range \( \lambda < \lambda_c \). The case is different when approaching the divergence from the case-2 region, where the perpendicular occupation tends to a finite number. The values \( \gamma = 1 \) and \( \beta = 1 \) were taken to produce the graphs in the right panel.

mixed state whose most important characterization is given by the grand canonical partition function

\[
\Xi = \sum_{M=0}^{\infty} \text{Tr} \left( e^{-\beta H_M - \mu M} \right).
\]

The presence of non-quadratic terms in the Hamiltonian hinders the exact analytical calculation of \( \Xi \). Hence, the following quadratic form is proposed

\[
\Xi \approx 1 + \frac{1}{\sqrt{\pi}} \sum_{M=1}^{\infty} e^{\frac{\beta M}{2}} \int_{-\infty}^{\infty} dx \ e^{-x^2} \text{Tr} \left( e^{-\beta (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + i \beta \gamma (\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1) + x \sqrt{\frac{2\pi}{\beta}} \left( \hat{m}_1 - \hat{m}_2 \right) + \beta \mu M} \right).
\]

The original grand partition function can be obtained from this expression by carrying out the integral treating operators as scalars. This procedure can be seen as a Hubbard–Stratonovich transformation [25] but without operator ordering. Expression (11) is expected to be accurate over parameter zones where the system displays high occupation, since in this case fluctuations become negligible compared to mean values. This has been observed through a numerical analysis in reference [24] in a closely related model. As can be seen from appendix B, in the process of calculating (11) it is found that \( \Xi \) converges inside the parameter zones highlighted in the left panel of figure 1. In the range \((-\infty, \lambda_D) \times (-\infty, \mu_D)\) the gran-partition function is given by

\[
\Xi = \frac{\xi(\lambda, \mu, \beta)}{(\lambda_D - \lambda) \kappa(\lambda) + \mu_D - \mu}.
\]

Variables \( \xi \) and \( \kappa \) as well as constant \( \alpha \) and the relation between \( \lambda_D \) and \( \mu_D \) are given in table 1. The grand partition function tends to diverge as any point of the curve \((\lambda_D, \mu_D)\) is approached.
Table 1. Constants related to the grand partition function in (12).

| Parameter | Expression |
|-----------|------------|
| $\lambda_c$ | $\sqrt{1 + \gamma^2}$ |
| $\lambda_D$ | $-2(\lambda_c + \mu_D)$ if $\mu_D \geq -\frac{3}{2} \lambda_c$, $\frac{1}{2} \left( -\mu_D + \sqrt{\mu_D^2 - 2\lambda_D^2} \right)$ if $\mu_D \leq -\frac{3}{2} \lambda_c$ |
| $\kappa(\lambda)$ | $\frac{1}{2} \lambda_c^2$ if $\lambda_D \leq \lambda_c$, $1 - \frac{\lambda_c^2}{2\lambda_D}$ if $\lambda_D \geq \lambda_c$ |
| $\alpha$ | $\frac{5}{4}$ if $(\lambda_D, \mu_D) = \left( \lambda_c, -\frac{3}{2} \lambda_c \right)$ |
| $\xi$ | A function of $\lambda, \mu$ and $\beta$ that tends to a finite value when $(\lambda, \mu) \rightarrow (\lambda_D, \mu_D)$ |

from the left. The line $\lambda = \lambda_c$ partitions the parameter space into cases whose properties are being discussed further ahead in this note. However, there is no symmetry breaking. In both cases the number of particles at both wells is the same. This can be seen from numerics but it also follows from the fact that the thermodynamic state is a function of the Hamiltonian as such it must reflect its symmetries. A number of observables can be obtained as derivatives of the grand partition function. These can be seen in table 2. They all show the same scaling behavior near divergence, namely, proportional to the total number of particles [26]. However, multiplicative coefficients display different functionality depending on the region of parameter space from which the divergence is approached. In general, it can be appreciated that at finite temperature the parameter space is divided into two cases that can be recognized according to the relations between physical observables. For instance, according to table 2 the relation between energy and mean number of particles is $E = \mu_D \mathcal{M}$, which displays a different behavior on each zone of figure 1 because $\mu_D$ has distinct functionalities depending on whether $\lambda$ is less or greater than $\lambda_c$. As simultaneous measurements of $E$ and $\mathcal{M}$ are possible because the Hamiltonian commutes with the operator that determines the mean number of particles, it follows $\mu_D$ could be obtained from such measurements. Likewise, constant $\lambda_D$ can be found by finding the value of $\lambda$ for which the equilibrium state collapses. In this way, mapping $\mu_D$ as a function of $\lambda_D$ it should be possible to identify the region of parameter space from which the divergence is being approached. Moreover, this behavior is being driven by the characteristic features of the zero-temperature response which define different phases on each side of the critical point $\lambda_c$. However, the precursors of the finite-temperature response must be of a different nature because under the action of a chemical potential the number of particles is being controlled and the system lacks symmetry-breaking mechanisms that would allow to spontaneously contravene its inversion symmetry. The subsequent analysis is intended to show that in this case what actually characterizes the thermodynamic state is its condensation potential. Specifically, the family of parameters for which there exists a symmetric phase at zero temperature determines a zone where a condensate can be formed, while the family of parameters associated with the broken phase determines a zone where condensation is inhibited.

3. Population distribution

Knowing that observables diverge when the system’s parameters approach an established boundary in parameter space, it is of interest to uncover some of the features that
Table 2. Mean values calculated over the grand-canonical ensemble. Mean number of particles $\mathcal{M}$, energy $E$, mean value of interaction $J$, mean value of phase- and phaseless-hopping, $J$ and $W$ respectively. Unreferenced variables are identified in table 1.

| Observable | Formal expression | Leading term close to $(\lambda_\text{D}, \mu_\text{D})$ | Functionality ($\times \mathcal{M}$) |
|------------|-------------------|--------------------------------------------------|--------------------------------|
| $\mathcal{M} = \langle \hat{m}_1 + \hat{m}_2 \rangle$ | $\frac{1}{\beta} \frac{\partial \log \Xi}{\partial \mu}$ | $\frac{\mu_\text{D} \mathcal{M}}{\beta} (\lambda_\text{D} - \lambda) + \mu_\text{D} - \mu$ | 1 |
| $E = \langle \hat{H} \rangle$ | $\mu_\text{D} \mathcal{M} - \frac{\beta}{\mu} \log \Xi$ | $-\lambda_\text{c} - \frac{\lambda_\text{D}}{2}$ | if $\lambda_\text{D} \leq \lambda_\text{c}$, |
| $I = \langle \frac{1}{M} \lambda_\text{D} m_1^2 + m_2^2 \rangle$ | $\frac{1}{\beta} \frac{\partial \log \Xi}{\partial \lambda}$ | $\kappa(\lambda_\text{D}) \mathcal{M}$ | $-\lambda_\text{D} - \frac{\lambda_\text{D}^2}{2\lambda_\text{D}}$ | if $\lambda_\text{D} \geq \lambda_\text{c}$ |
| $J = -i \langle \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1 \rangle$ | $- \frac{\beta}{\lambda} \frac{\partial \log \Xi}{\partial \gamma}$ | $\frac{\gamma(\lambda_\text{D})}{\lambda_\text{c}} \frac{\partial \lambda_\text{D}}{\partial \lambda_\text{c}} \mathcal{M}$ | $-\frac{\gamma}{\lambda_\text{c}}$ | if $\lambda_\text{D} \leq \lambda_\text{c}$, |
| $W = \langle \hat{a}_1 \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 \rangle$ | $E - \gamma J + \lambda \left[ \mu_\text{D} + \kappa(\lambda_\text{D}) \left( \lambda_\text{D} - \frac{\lambda_\text{D}^2}{\lambda_\text{D}} \right) \right] \mathcal{M}$ | $E$ | $\frac{1}{\lambda_\text{D}}$ | if $\lambda_\text{D} \geq \lambda_\text{c}$ |

characterize the thermodynamic state near this divergence zone. One way of addressing this issue is to find how much a given mode contributes to the thermodynamic state. Although bosons can access two independent modes, one for each well in Hamiltonian (1), it is possible to build other (linearly dependent) modes as superpositions of the original ones. In this scenario it becomes relevant to find the mean occupation of a given mode. For this purpose let us define the following weight function

$$N(\theta, \varphi) = \langle \hat{b}^\dagger \hat{b} \rangle, \quad \hat{b}^\dagger = \hat{a}_1^\dagger \cos \theta - \hat{a}_2^\dagger \sin \theta.$$  \hspace{1cm} (13)

The average is calculated over the thermodynamic state associated with the grand partition function previously introduced in this document. Any mode available in physical space can be reached in the range $0 \leq \theta \leq \pi/2$ and $0 \leq \varphi < 2\pi$. From a direct calculation it can be shown that this weight function can also be written as

$$N = \frac{\mathcal{M}}{2} - \frac{\sin 2\theta}{2} (W \cos \varphi + J \sin \varphi).$$  \hspace{1cm} (14)

In the process of arriving at this expression the property $\langle \hat{m}_1 - \hat{m}_2 \rangle = 0$ was used. This property follows from the fact that the equilibrium state must display the Hamiltonian’s inversion symmetry. An explicit form of $N$ can be obtained by replacing the mean values of table 2 in (14). A pair of angles $(\theta^*, \varphi^*)$ defining a mode with maximum contribution must fulfill

$$\partial_\theta N|_{\theta^*, \varphi^*} = - \cos 2\theta^* (W \cos \varphi^* + J \sin \varphi^*) = 0, \hspace{1cm} \text{(15)}$$
$$\partial_\varphi N|_{\theta^*, \varphi^*} = \sin 2\theta^* (W \sin \varphi^* - J \cos \varphi^*) = 0, \hspace{1cm} \text{(16)}$$
$$\partial_{\theta^2} N|_{\theta^*, \varphi^*} = 2 \sin 2\theta^* (W \cos \varphi^* + J \sin \varphi^*) < 0, \hspace{1cm} \text{(17)}$$
\[ 4\partial^2 N_{\theta^\Lambda \phi^\Lambda} = \partial^2 N_{\theta^\Lambda \phi^\Lambda} < 0. \] (18)

As can be seen, condition (17) implies (18), so it is really three conditions that must be accounted for. Equation (15) is met for \( \theta^\Lambda = \pi/4 \), giving a state with equal occupation at both sides, in compliance with the Hamiltonian’s symmetry. According to table 2 both \( W \) and \( J \) are negative in the zone near divergence, hence conditions (16) and (17) are satisfied for

\[ \cos \phi^\Lambda = \frac{1}{\sqrt{1 + t^2}}, \quad \sin \phi^\Lambda = \frac{t}{\sqrt{1 + t^2}}, \quad t = \frac{J}{W} = \gamma. \] (19)

Interestingly, these parameters also define the ground state in the gapped phase \( \lambda < \lambda_c \) of the quantum phase transition discussed in the first part of this work, but in this case this state with maximum occupation applies to the whole spectrum of parameters near divergence, including the gapless phase. The maximum occupation number is given by

\[ N^\Lambda = N(\theta^\Lambda, \phi^\Lambda) = \frac{M}{2} + \frac{1}{2} \sqrt{W^2 + J^2}. \] (20)

Inserting the values reported in table 2 it results

\[ n = \frac{N^\Lambda}{M} = \begin{cases} 1 & \text{if } \lambda_D \leq \lambda_c, \\ \frac{1}{2} \left(1 + \frac{\lambda_c}{\lambda_D}\right) & \text{if } \lambda_D \geq \lambda_c. \end{cases} \] (21)

As below \( \lambda_c \) the number of particles in the most populated mode coincides with the mean number of particles in the whole system, it is argued that in this regime particles go all into the maximally occupied mode, which is at the same time the ground state of the high-density Hamiltonian. The quantity

\[ n_\perp = 1 - n, \] (22)

is also the relative mean number of particles in the mode perpendicular to \( \hat{b}^\dagger, \hat{a}^\dagger = \hat{a}_1^\dagger \cos \theta + \hat{a}_2^\dagger e^{i\phi} \sin \theta \), evaluated at \( (\theta^\Lambda, \phi^\Lambda) \). It then follows that for the case-1 family of parameters in the left panel of figure 1 the number of particles in the maximally occupied state approaches the mean number of particles in the system at the same time that the number of particles in the respective perpendicular state becomes negligible. Instead, in the case-2 region the population is distributed over two modes. Take into account that this derivation is valid near the curve of divergence and not necessarily over the whole space of parameters.

A numerical study is undertaken in order to benchmark these analytical results. Hamiltonian (1) is diagonalized for various system sizes \( M \) and the respective eigenvalues \( E_j^M \) are used to find the grand canonical partition function thus

\[ \Xi = 1 + \sum_{M=1}^{M_{\text{as}}} e^{\beta M} \sum_{j=1}^{M+1} e^{-\beta E_j^M}. \] (23)

The maximum size \( M_{\text{as}} \) is adjusted depending on the system’s parameters to achieve a relative accuracy of \( \Delta \Xi/\Xi < 10^{-7} \). Eigenvalues can be in addition employed to calculate the mean number of particles \( \langle M \rangle \) using a similar expression. Eigenvectors are also calculated and used to find \( J \) and \( W \) as weighed sums (not as numerical derivatives) in similarity to (23). These values are then used to find \( n_\perp \). The results are shown in the right panel of figure 1.
The numerical values of $n_\perp$ show a tendency that is consistent with the analytical study, displaying a monotonously decaying pattern as the divergence is approached by either $\lambda$ or $\mu$ from the case-1 region. The same tendency is observed when the divergence is approached through the line that divides the parameter space. From a numerical analysis it has been determined that the decaying is stronger when approaching $(\lambda_D, \mu_D) = (\lambda_c, -\frac{3}{2}\lambda_c)$ (black and red curves), scaling as $\approx x^{0.020\pm0.001}$ close to the origin. In other cases the decaying coefficient is smaller and seems to be dependent on the divergence point. Furthermore, $n_\perp$ grows when approaching $\lambda_D$ or $\mu_D$ at close range from the case-2 region, suggesting a macroscopic fraction of particles settle in the perpendicular mode. These features show that the properties of the high-density ground state dominate the collective response in thermodynamic equilibrium [27]. However, the observed behavior at finite temperature does not fit into a phase transition scheme just like the zero temperature response does. Instead, the gapped phase of the zero-temperature system transmutes into a collective state at finite temperature in which bosons cluster together in a single mode. The intensity of this coalescence is enhanced by the proximity of interaction and chemical potential to the divergence region. The effect of temperature on this process seems rather marginal, but by establishing a parallel with the analogous situation on the interactionless condensate [1] one can argue that a macroscopic occupation can be defined below certain temperature. This part is skipped in this work because the procedure involves phenomenological considerations that might depend on specifics. The fact that compressibility, which can be found as $\partial_\mu M$, goes to infinity in general as $(\lambda, \mu) \to (\lambda_D, \mu_D)$ is indicative of a highly conductive state not necessarily correlated with collectivism. As a final note, it is relevant to mention how these results contrast with existing studies on attractive condensates [2–12]. Such studies often report that attractive interaction is seen to lead to instability. This behavior is compatible with what is expected in systems on a high interaction regime, i.e., when $\lambda > \lambda_c$. The central consideration to take into account is that here the interaction constant has been rescaled with respect to the number of particles (equation (1)). As a consequence, systems governed by Hamiltonians with unrescaled constants necessarily fall into the high-interaction regime because without rescaling the interaction part of the Hamiltonian takes over. A fundamental result of the present research is therefore that in order to produce a stable condensate with attractive interactions the Hamiltonian parameters should be engineered to produce single- and many-body contributions with the same scaling.

4. Conclusions

The equilibrium response of a bosonic system displaying a quantum phase transition has been studied using the grand canonical formalism. The phases characterizing the zero-temperature state drive characteristic features in the finite temperature regime near the parameter zone where the partition function diverged. A form of quantum collectivism in which occupation is concentrated in the ground-state mode has been identified. Too much attraction tends to dissolve this state, but there exist a critical value of the interaction constant below which collectivism can prevail in the presence of attractive interaction. This is related to the effect that the negative chemical potential considered here has on balancing the instability caused by the attractive interaction and the fact that the interaction constant has been rescaled with respect to the system size. Moreover, according to the phase diagram in figure 1 there cannot be a condensed phase for positive values of the chemical potential. Perhaps the most critical aspect of the present study is therefore the consideration of negative chemical potential, which might pose technical challenges in a controlled scenario [28], but could take place spontaneously in a less-artificial one, as for example a bosonic superfluid. It remains to be seen whether other
forms of collectivism can be induced by deliberately breaking the system’s inversion symmetry, for instance, by setting different chemical-potential variables at each well. Also of interest is to scale up the model by considering a large number of modes in one dimension and see whether the collectivism observed in the small system can be a precursor of condensation in an infinite chain. Ultimately, by adding bosonic modes describing molecules it should be possible to study the interplay between attractiveness and molecular formation.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Appendix A. Quantum phase transition

Making $\delta = 1$ Hamiltonian (1) becomes

$$\hat{H}_M = \hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 - i\gamma (\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1) - \frac{\lambda}{M} \left( \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1^\dagger + \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2^\dagger \right). \quad (A1)$$

It is assumed that the ground state can be written as

$$|G(\theta, \varphi)\rangle = \frac{\hat{b}_1^M|0,0\rangle}{\sqrt{M!}} = |M,0\rangle, \quad (A2)$$

$$\hat{b}_1^1 = \hat{a}_1^\dagger \cos \theta - \hat{a}_2^\dagger e^{i\varphi} \sin \theta, \quad (A3)$$

so that $[\hat{b}_1, \hat{b}_1^\dagger] = 1$. The angle domains are $0 \leq \theta \leq \frac{\pi}{2}$ and $0 \leq \varphi < 2\pi$, in such a way that different angle pairs correspond to different modes. The basis change is given by

$$\begin{bmatrix} \hat{b}_1 \\ \hat{b}_2 \end{bmatrix} = \begin{bmatrix} \cos \theta & -e^{i\varphi} \sin \theta \\ e^{-i\varphi} \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} \quad (A4)$$

$$\Rightarrow \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} = \begin{bmatrix} \cos \theta & e^{i\varphi} \sin \theta \\ -e^{-i\varphi} \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} \hat{b}_1^1 \\ \hat{b}_2^1 \end{bmatrix}. \quad (A5)$$

From direct calculations the following results are obtained

$$\langle G|\hat{a}_1^\dagger \hat{a}_2|G\rangle = -M e^{i\varphi} \cos \theta \sin \theta, \quad (A6)$$

$$\langle G|\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1|G\rangle = M^2 \cos^4 \theta + M \cos^2 \theta \sin^2 \theta, \quad (A7)$$

$$\langle G|\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2|G\rangle = M^2 \sin^4 \theta + M \cos^2 \theta \sin^2 \theta. \quad (A8)$$
Using these values the energy becomes to leading order in $M$

$$E_G(\theta, \varphi) = \langle G(\theta, \varphi) | i \hat{H} G(\theta, \varphi) \rangle = -M \left( \sin 2\theta (\cos \varphi + \gamma \sin \varphi) + \lambda \left( 1 - \frac{\sin^2 2\theta}{2} \right) \right).$$

(A9)

The ground state energy corresponds to the minimum of this expression with respect to $\theta$ and $\varphi$. Defining

$$q(\theta, \varphi) = \sin 2\theta (\cos \varphi + \gamma \sin \varphi) - \frac{\lambda \sin^2 2\theta}{2},$$

(A10)

extreme points must satisfy

$$\partial_{\theta} q|_{\theta^*, \varphi^*} = \cos 2\theta^* (\cos \varphi^* + \gamma \sin \varphi^* - \lambda \sin 2\theta^*) = 0,$$

(A11)

$$\partial_{\varphi} q|_{\theta^*, \varphi^*} = -\sin 2\theta^* (\sin \varphi^* - \gamma \cos \varphi^*) = 0,$$

(A12)

$$\partial^2_{\varphi} q|_{\theta^*, \varphi^*} = -2 \sin 2\theta^* (\cos \varphi^* + \gamma \sin \varphi^* - \lambda \sin 2\theta^*) - \lambda \cos^2 2\varphi^* < 0,$$

(A13)

$$\partial^2_{\theta} q|_{\theta^*, \varphi^*} = \sin 2\varphi^* (\cos \varphi^* - \gamma \cos \varphi^*) < 0.$$  

(A14)

Conditions (A11), (A12) and (A14) are all met for the next values

$$\theta^* = \frac{\pi}{4}, \quad \cos \varphi^* = \frac{1}{\sqrt{1 + \gamma^2}}, \quad \sin \varphi^* = \frac{\gamma}{\sqrt{1 + \gamma^2}}.$$  

(A15)

Condition (A13) is met for these same values in the range $\lambda < \sqrt{1 + \gamma^2}$, which defines the scope of this particular physical phase. Replacing these extreme points in (A9) the ground state energy in this phase is found to be

$$E_G = -M \left( \sqrt{1 + \gamma^2} + \frac{\lambda}{2} \right).$$  

(A16)

Correspondingly, over the range $\lambda > \sqrt{1 + \gamma^2}$ the following values constitute solutions

$$\theta_1^* = \frac{1}{2} \arcsin \frac{\sqrt{1 + \gamma^2}}{\lambda}, \quad \theta_2^* = \frac{\pi}{2} - \theta_1^*,$$

(A17)

$$\cos \varphi^* = \frac{1}{\sqrt{1 + \gamma^2}}, \quad \sin \varphi^* = \frac{\gamma}{\sqrt{1 + \gamma^2}}.$$  

(A18)

The solutions are given by the pairs $\{\theta_1^*, \varphi^*\}$ and $\{\theta_2^*, \varphi^*\}$. Either pair delivers the following ground state energy

$$E_G = -M \left( \lambda + \frac{1 + \gamma^2}{2\lambda} \right).$$  

(A19)

The expression

$$\lambda_c = \sqrt{1 + \gamma^2},$$  

(A20)
is the transition’s critical point. Since these results correspond to first order in $M$, the quantum phase transition takes place in the high density limit, i.e., $M \to \infty$. Because the energy is continuous at the critical point, it is argued that this is a second order transition. The order parameter measures the degree of symmetry breaking and for this it is good to consider the difference in occupation at the system’s sites

$$\Delta = \left( \frac{\langle \hat{a}^+ \hat{a}_1 - \hat{a}^+_2 \hat{a}_2 \rangle}{M} \right)^2 = \begin{cases} 0 & \text{if } \lambda \leq \lambda_c, \\ 1 - \frac{\lambda}{\lambda_c} & \text{if } \lambda \geq \lambda_c. \end{cases} \quad (A21)$$

### Appendix B. Calculation of $\Xi$

Taking equation (11) and making the variable change $x = y\sqrt{M}\beta$ leads to the next expression

$$\Xi \approx 1 + \frac{1}{\pi} \sum_{M=1}^{\infty} \sqrt{M} \, e^{\frac{\beta M}{2}} \int_{-\infty}^{\infty} dy \, e^{-\beta M y^2} \, \text{Tr}(e^{\hat{b}^\dagger \hat{b}}), \quad (B1)$$

so that

$$\hat{h}_M = -\langle \hat{a}_1 \hat{a}_2 + \hat{a}_2^+ \hat{a}_1 \rangle + i\gamma (\hat{a}_1 \hat{a}_2 - \hat{a}_2^+ \hat{a}_1) + \sqrt{2\lambda y(y_1 - y_2) + \mu(y_1 + y_2)}.$$ \quad (B2)

This effective Hamiltonian can also be written as

$$\hat{h}_M = (\hat{a}_1^+ \hat{a}_2^+ \mu + \sqrt{2\lambda y} - 1 + i\gamma \mu - \sqrt{2\lambda y} \hat{a}_1 \hat{a}_2). \quad (B3)$$

Normal eigenenergies of $\hat{h}_M$ are then found to be

$$\epsilon_{\pm}(y) = \mu \pm \sqrt{2\lambda y^2 + 1 + \gamma^2} = \mu \pm \sqrt{2\lambda y^2 + \lambda_c^2}.$$ \quad (B4)

Using these values the trace can be calculated as follows

$$\text{Tr}(e^{\beta \hat{b}^\dagger \hat{b}}) = \text{Tr}(e^{\beta_{(e^+)}\beta_{(e^-)}\hat{b}^+ + \epsilon_{(e^+)}\hat{b}^+ \hat{b}^- + \epsilon_{(e^-)}\hat{b}^-}) = \sum_{n=0}^{\infty} e^{\beta_{(e^+)}n + \beta_{(e^-)}(M-n)} = \frac{e^{\beta_{(e^-)} - e^{\beta_{(e^+)} - \epsilon_{(e^-)}}} e^{\beta_{(e^+)}M}}{1 - e^{\beta_{(e^-)} - \epsilon_{(e^-)}}}. \quad (B5)$$

Operators $\hat{b}^+_{\pm}$ and $\hat{b}^-_{\pm}$ correspond to diagonal bosonic modes. Now let us take a term from (B1) and reformulated in the next way

$$\sqrt{M} \, e^{\frac{\beta M}{\sqrt{\pi}}} = \sqrt{M} \int_{-\infty}^{\infty} dx \, e^{-\beta \sqrt{M} x^2 + \beta \sqrt{M} \sqrt{2\lambda y}}.$$ \quad (B6)

Replacing (B5) and (B6) in (B1) and organizing terms yields

$$\Xi = 1 + \frac{\beta}{\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \sum_{M=1}^{\infty} M e^{\beta M (-x^2 - y^2 + \sqrt{2\lambda y} + c_+(y))} \frac{1 - e^{-\beta (c_+(y) - c_-(y))}}{1 - e^{\beta (c_+(y) - c_-(y))}}$$

$$+ \sum_{M=1}^{\infty} M e^{\beta M (-x^2 - y^2 + \sqrt{2\lambda y} + c_-(y))} \frac{1 - e^{\beta (c_+(y) - c_-(y))}}{1 - e^{-\beta (c_+(y) - c_-(y))}}.$$ \quad (B7)
Defining
\[ F(x, y) = -x^2 - y^2 + \sqrt{2\lambda x} + \sqrt{2\lambda y^2} + \lambda^2 + \mu, \tag{B8} \]
it can be seen that both sums in (B7) shall converge if \( F(x, y) < 0 \) for any real value of \( x \) and \( y \). For this it is necessary that
\[ F(x^*, y^*) = F^* < 0, \tag{B9} \]
where \( x^* \) and \( y^* \) demark the location of the function’s global maximum. Through a calculus analysis it can be shown that two main cases arise

\textbf{B.1. Case 1:} \( 0 \leq \lambda < \min(-2(\mu + \lambda_c), \lambda_c) \)

The function’s only maximum is located at \( (x^* = \sqrt{\lambda/2}, y^* = 0) \). The system’s parameters are compatible with the condition
\[ F^* = \frac{\lambda}{2} + \lambda_c + \mu = -\frac{\lambda_D - \lambda}{2} - (\mu_D - \mu) < 0, \tag{B10} \]
being \( \lambda_D \) and \( \mu_D \) a pair of constants satisfying \( \lambda_D = -2(\lambda_c + \mu_D) \). Equation (B10) highlights the fact that
\[ \lim_{\lambda \to \lambda_D, \mu \to \mu_D} F^* = 0. \tag{B11} \]

\textbf{B.2. Case 2:} \( \lambda_c > -\frac{3}{2} \) and \( \lambda_c \leq \lambda < \frac{1}{2} \left( -\mu + \sqrt{\mu^2 - 2\lambda_c^2} \right) \)

The function displays two maxima located at
\[ \left( x^* = \sqrt{\frac{\lambda}{2}}, y^* = \sqrt{\frac{2\lambda^2 - \lambda_c^2}{2\lambda}} \right), \tag{B12} \]
and
\[ \left( x^* = \sqrt{\frac{\lambda}{2}}, y^* = -\sqrt{\frac{2\lambda^2 - \lambda_c^2}{2\lambda}} \right). \tag{B13} \]

The system’s parameters are compatible with the condition
\[ F^* = \lambda + \frac{\lambda_c^2}{2\lambda} + \mu = -(\lambda_D - \lambda) \left( 1 - \frac{\lambda_c^2}{2\lambda_D^2} \right) - (\mu_D - \mu) < 0, \tag{B14} \]
such that \( \lambda_D = \frac{1}{\frac{2}{\mu_D^2 - 2\lambda_c^2}} \). As in the previous case, equation (B11) is satisfied. Figure 1 depicts the two cases in a parameter map. The divergence parameters, \( (\lambda_D, \mu_D) \), are related as follows
\[ \lambda_D = \begin{cases} -2(\lambda_c + \mu_D) & \text{if } \mu_D \geq -\frac{3}{2}\lambda_c, \\ \frac{1}{2} \left( -\mu_D + \sqrt{\mu_D^2 - 2\lambda_c^2} \right) & \text{if } \mu_D \leq -\frac{3}{2}\lambda_c. \end{cases} \tag{B15} \]
Solving the sums in (B7) within the established spaces of convergence the following result is obtained
\[
\Xi \approx 1 + \frac{\beta}{4\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{\text{csch}^2 \left( \frac{\beta}{2} F(x, y) \right)}{1 - e^{-\beta \sqrt{\phi} y}} + \frac{\text{csch}^2 \left( \frac{\beta}{2} G(x, y) \right)}{1 - e^{\beta \sqrt{\phi} y}}.
\]  
(B16)

where
\[
G(x, y) = F(x, y) - \sqrt{y}, \quad \sqrt{y} = 2\sqrt{2\lambda y^2 + \lambda_c^2}.
\]  
(B17)

Close to divergence, only the part of the integral with \( F(x, y) \) in (B16) goes to infinity. Since in such a case \( F(x, y) \) gets close to zero, the following approximation becomes applicable
\[
\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{\text{csch}^2 \left( \frac{\beta}{2} F(x, y) \right)}{1 - e^{-\beta \sqrt{\phi} y}} \approx \frac{4}{\beta^2} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{e^{\beta F(x, y)}}{F(x, y)^2(1 - e^{-\beta \sqrt{\phi} y})}.
\]  
(B18)

Neither exponential in the integrand has a significant contribution to the scaling pattern of the grand-partition function. Therefore, the integral is further approximated by
\[
\frac{4 e^{\beta F^*}}{\beta^2(1 - e^{-\beta \sqrt{\phi} y})} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{1}{F(x, y)^2}.
\]  
(B19)

The integral above can be approximated close to the divergence zone, but for this it is necessary to differentiate a number of subcases.

**B.3. Case 1: \( 0 < \lambda < \min(-2(\mu + \lambda_c)) \)**

**B.3.1. Subcase 1: excluding \( (\lambda_D, \mu_D) = (\lambda_c, -\frac{3\lambda_c}{2}) \).** Function \( F(x, y) \) is expanded and the first nonvanishing terms are retained. The resulting integral can be solved by standard methods, along the lines of
\[
\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{1}{F(x, y)^2} \approx \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{1}{(F^* - \alpha_x^2(x-x^*)^2 - \alpha_y^2(y-y^*)^2)^2} = -\frac{\pi}{|\alpha_x||\alpha_y|F^*},
\]  
(B20)

being
\[
\alpha_x^2 = -\frac{1}{2} \frac{\partial^2 F}{\partial x^2} \bigg|_{x=x^*,y=y^*}, \quad \alpha_y^2 = -\frac{1}{2} \frac{\partial^2 F}{\partial y^2} \bigg|_{x=x^*,y=y^*}.
\]  
(B21)

An approximated expression to the grand partition function can be obtained by gathering all the coefficients involved in the derivation. However, it is only the denominator in the last term of (B20) that determines the divergence trend. The resulting expression is valid inside the parameter zone corresponding to this case. Replacing the following identities in (B20):
\[
F^* = -\frac{(\lambda_D - \lambda)}{2} - (\mu_D - \mu), \quad \alpha_x^2 = 1, \quad \alpha_y^2 = 1 - \frac{\lambda}{\lambda_c},
\]  
(B22-24)
the grand-partition function can be written as

$$\Xi = \frac{\xi(\lambda, \mu, \lambda_c)}{\lambda - \lambda_c + \mu - \mu}.$$  \hfill (B25)

Function $\xi(\lambda, \mu, \lambda_c)$ must be well behaved and continuous at the point $(\lambda, \mu) = (\lambda_D, \mu_D)$. The reason why this derivation cannot accommodate $\lambda_D = \lambda_c$ is because this would allow $\lambda$ to get infinitesimally close to $\lambda_c$, causing the vanishing of $\alpha_y$ in (B24).

**B.3.2. Subcase 2**: $(\lambda_D, \mu_D) = (\lambda_c, -\frac{3\lambda_c}{2})$. As one of the second-order expansion-terms of $F(x, y)$ vanishes when $\lambda$ approaches $\lambda_c$, the next non-vanishing term of the expansion is considered in (B20). The resulting expression reads

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \left( F^* - \alpha_x^2(x - x)^2 - \gamma_y^2(y - y^2)^4 \right) \frac{1}{(\lambda - \lambda_c + \mu - \mu)}.$$  \hfill (B26)

Replacing

$$F^* = -\frac{(\lambda_c - \lambda)}{2} \left( -\frac{3\lambda_c}{2} - \mu \right),$$  \hfill (B27)

$$\alpha_x^2 = 1,$$  \hfill (B28)

$$\gamma_y^2 = \frac{\lambda^2}{2\lambda_c^2}.$$  \hfill (B29)

As a consequence, the grand partition function adopts the next form

$$\Xi = \frac{\xi(\lambda, \mu, \lambda_c)}{(\lambda - \lambda_c - \frac{3\lambda_c}{2} - \mu)}.$$  \hfill (B30)

in such a way that $\xi(\lambda, \mu, \lambda_c)$ be well behaved and continuous at $(\lambda, \mu) = (\lambda_c, -\frac{3\lambda_c}{2})$.

**B.4 Case 2**: \( \frac{\lambda_c}{2} < - \frac{3}{2} \) and \( \lambda_c \leq \lambda < \frac{1}{2} \left( -\mu + \sqrt{\mu^2 - 2\lambda_c^2} \right) \)

**B.4.1. Subcase 3: excluding** $(\lambda_D, \mu_D) = (\lambda_c, -\frac{3\lambda_c}{2})$. In this case function $F(x, y)$ has two maxima located at opposite sides of the $y$ axis. Formally, this would require to consider the contribution of two expansions, deriving in two integrals, each of which limited to half the plane.

However, due to the symmetry of $F(x, y)$, this is effectively equivalent to considering twice one expansion integrated over the whole plane, since only the contribution around the expansion point is relevant. Proceeding in this way, the same expression (B20) found before is obtained. Likewise, replacing

$$F^* = -\left( \frac{\lambda_c}{2} - \lambda \right) \left( 1 - \frac{\lambda^2}{2\lambda_D^2} \right) - (\mu - \mu_D),$$  \hfill (B31)

$$\alpha_x^2 = 1,$$  \hfill (B32)

$$\alpha_y^2 = 1 - \left( \frac{\lambda_c}{\lambda} \right)^2.$$  \hfill (B33)
it follows that the grand partition function can be written as

$$\Xi = \frac{\xi(\lambda, \mu, \lambda_c)}{(\lambda_D - \lambda) \left( 1 - \frac{\lambda^2}{2\lambda_D} \right) + (\mu_D - \mu)},$$

(B34)

being $\xi(\lambda, \mu, \lambda_c)$ a well behaved and continuous function at $(\lambda, \mu) = (\lambda_D, \mu_D)$.

**B.4.2. Subcase 4:** $(\lambda_D, \mu_D) = (\lambda_c, -\frac{3}{2} \lambda_c)$. In close parallel to subcase 2, function $F(x,y)$ is expanded and the first non-vanishing terms that survive in the limit $\lambda \to \lambda_c$ are retained. The resulting expression coincides with (B26). Replacing

$$F^* = -\frac{\lambda_c}{2} - \left( -\frac{3}{2} \lambda_c - \mu \right),$$

(B35)

$$\alpha_i^2 = 1,$$  \hspace{1cm} \hspace{1cm} (B36)

$$\gamma_i^2 = \frac{\lambda_c^2}{2\lambda} \left( \lambda_c^2 - 4(\lambda^2 - \lambda_c^2) \right),$$

(B37)

the final form of the grand-partition function is found to be analogous to (B30). The grand partition function can be written in a general way as

$$\Xi = \frac{\xi}{[(\lambda_D - \lambda)\kappa(\lambda) + \mu_D - \mu]^\alpha}.$$  \hspace{1cm} (B38)

Function $\xi$ does not contribute to the scaling pattern of $\Xi$ and makes no significant contribution to observables in the parameter zone near divergence. The other variables are given by

$$\kappa(\lambda) = \begin{cases} 
\frac{1}{2} & \text{if } \lambda_D \leq \lambda_c, \\
1 - \frac{\lambda^2}{2\lambda_D} & \text{if } \lambda_D \geq \lambda_c,
\end{cases}$$

(B39)

and

$$\alpha = \begin{cases} 
1 & \text{if } (\lambda_D, \mu_D) \neq \left( \lambda_c, -\frac{3}{2} \lambda_c \right), \\
\frac{5}{4} & \text{if } (\lambda_D, \mu_D) = \left( \lambda_c, -\frac{3}{2} \lambda_c \right).
\end{cases}$$

(B40)

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