The pathway toward the formation of supermixed states in ultracold boson mixtures loaded in ring lattices

Andrea Richaud and Vittorio Penna

Dipartimento di Scienza Applicata e Tecnologia and u.d.r. CNISM, Politecnico di Torino, Corso Duca degli Abruzzi 24, I-10129 Torino, Italy

(Dated: March 25, 2019)

We investigate the mechanism of formation of supermixed soliton-like states in bosonic binary mixtures loaded in ring lattices. We evidence the presence of a common pathway which, irrespective of the number of lattice sites and upon variation of the interspecies attraction, leads the system from a mixed and delocalized phase to a supermixed and localized one, passing through an intermediate phase where the supermixed soliton progressively emerges. The degrees of mixing, localization and quantum correlation of the two condensed species, quantified by means of suitable indicators commonly used in Statistical Thermodynamics and Quantum Information Theory, allow one to reconstruct a bi-dimensional mixing-supermixing phase diagram featuring two characteristic critical lines. Our analysis is developed both within a semiclassical approach capable of capturing the essential features of the two-step mixing-demixing transition and with a fully-quantum approach.

I. INTRODUCTION

In the last decade, a considerable attention has been paid to the mixing-demixing transitions occurring in bosonic binary mixtures confined in optical lattices. Such systems, realized by means of both homonuclear [1] and heteronuclear [2] components, show how the interplay among the intra-species and the inter-species repulsion, the tunneling effect and the fragmentation induced by the periodic potential strongly affects the mixing properties and gives rise to an extremely rich phenomenology. This includes spatial phase separation in large-size lattices [3, 4], mixing properties of dipolar bosons [5], quantum emulsions [6, 7], the structure of quasiparticle spectrum across the demixing transition [8], and the influence on phase separation of thermal effects [9], interspecies entanglement [10], and asymmetric boson species [11]. Further aspects concerning the interlink between demixing and the dynamics of mixtures have been explored in [12–15].

Recently, spatial phase separation has been investigated for repulsive interspecies interactions in small-size lattices [16–19]. This analysis has disclosed an unexpectedly-complex demixing mechanism in which the regimes with fully-separated and the fully-mixed components are connected by an intermediate phase still exhibiting partial mixing. Overall, the resulting phases feature specific miscibility properties which can be quantified by means of the entropy of mixing, an indicator originally introduced in the context of macromolecular simulations [20]. The demixing of two quantum fluids, and their ensuing localization in different spatial domains, has been shown to be strictly linked with the presence of criticalities in several quantum indicators including, but not limited to, ground-state energy, energy levels’ structure and entanglement between the species [18, 21].

In this work, we aim at exploring the characteristic regimes of the mixture when the interaction between the condensed species is attractive. The competition between the interspecies attraction and the intraspecies repulsions results in a rather rich variety of phenomena which culminates in the formation of a supermixed soliton, i.e. a configuration where both condensed species localize in a unique site.

The scope of our analysis is rather broad, both because we take into account the possible presence of asymmetries between the condensed species and because the analysis itself is developed for a generic $L$-site trapping potential with ring geometry. A semiclassical scheme based on the approximation of inherently discrete quantum numbers with continuous variables (hence the name “continuous variable picture” (CVP)) allows one to reduce the original quantum problem to a classical one [22, 23]. The latter, in turn, displays, in a rather transparent way, the occurrence of critical phenomena such as the formation of soliton-like configurations and the onset of mixing-demixing or mixing-supermixing transitions.

Interestingly, our analysis not only highlights the fact that the formation of a supermixed soliton constitutes a two-step process, made possible by the non-linearity of the interspecies-attraction term, but also that this two-step process occurs in a generic $L$-site potential, no matter the specific value of $L$. In other words, depending on the strength of the interspecies attraction, but irrespective of the value of $L$, the system’s ground state exhibits three qualitatively different spatial structures: $i)$ the one featuring uniform boson distribution among all the wells, $ii)$ the one already including the seed of the supermixed soliton but featuring an incomplete localization and $iii)$ the one where the supermixed soliton is fully emerged and developed.

The phase diagram derived within this semiclassical approach is then validated by means of several genuinely quantum indicators, which indeed confirm the presence of three qualitatively different classes of ground states and the occurrence of a two-step process leading to the...
II. THE MODEL

A. The quantum model

In this article, we focus on the supermixing effect and on the soliton-formation mechanism in a two-component bosonic mixture loaded in $L$-site potentials. The genuinely quantum features of such system can be effectively captured by the second-quantized Hamiltonian

$$
H = -T_a \sum_{j=1}^{L} \left( a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1} \right) + \frac{U_a}{2} \sum_{j=1}^{L} n_j (n_j - 1) \\
- T_b \sum_{j=1}^{L} \left( b_{j+1}^\dagger b_j + b_j^\dagger b_{j+1} \right) + \frac{U_b}{2} \sum_{j=1}^{L} m_j (m_j - 1) \\
+W \sum_{j=1}^{L} n_j m_j,
$$

(1)

an extended version of the well-known Bose-Hubbard model whose last term accounts for the attractive interaction between the species. Operator $a_i$ ($b_i$) destroys a species a (species b) boson in the $i$-th site. Notice that $i \in \{1, \ldots, L\}$ and that, for $L > 2$, the trapping potential is assumed to feature a ring geometry, a circumstance which results in the periodic boundary conditions $i = L + 1 \equiv 1$. As a consequence of the bosonic character of the trapped particles, the following commutation relations hold: $[a_i, b_j^\dagger] = 0, [a_i^\dagger, a_j] = [b_i, b_j^\dagger] = \delta_{i,j}$. The definition of number operators, $n_i = a_i^\dagger a_i$ and $m_i = b_i^\dagger b_i$, allows one to evidence two independent conserved quantities, namely $N_a = \sum_i n_i$ and $N_b = \sum_i m_i$. Concerning model parameters, $T_a$ and $T_b$ represent the tunnelling energy of the two species, $U_a > 0$ and $U_b > 0$ their intra-species repulsive interactions, and $W < 0$ the inter-species attractive coupling.

B. A Continuous Variable Picture for the detection of different quantum phases

An effective way to determine the ground state structure of multimode BH Hamiltonians consists in approximating the inherently discrete single-site occupation numbers $n_j$ and $m_j$ with continuous variables $x_j = n_j/N_a$ and $y_j = m_j/N_b$ \cite{18, 19, 22, 24, 27, 28}. Provided that the overall boson populations, $N_a = \sum_j n_j$ and $N_b = \sum_j m_j$, are large enough, it is in fact possible to establish a one-to-one correspondence between a certain Fock state $|n_1, \ldots, n_L, m_1, \ldots, m_L\rangle = |\vec{n}, \vec{m}\rangle$ and state $|x_1, \ldots, x_L, y_1, \ldots, y_L\rangle = |\vec{x}, \vec{y}\rangle$, i.e. to turn integer quantum numbers $n_j$ and $m_j$ into real variables $x_j$ and $y_j$, both $\in [0,1]$. With this in mind, creation and annihilation processes $n_j \rightarrow n_j \pm 1$ ($m_j \rightarrow m_j \pm 1$) can be associated to small changes of the corresponding continuous variable, i.e. $x_j \rightarrow x_j \pm \epsilon_n$ ($y_j \rightarrow y_j \pm \epsilon_m$) where $\epsilon_n = 1/N_a \ll 1$ ($\epsilon_m = 1/N_b \ll 1$). The application of this approximation scheme to a second-quantized Hamiltonian of the type (1) allows one to reformulate it in terms of generalized coordinates $x_j$ and $y_j$ and of their conjugate momenta. As a consequence, within such scheme, the (quadratic approximation of the) eigenvalue problem $H|E\rangle = E|E\rangle$ reads

$$
(-\mathcal{D} + \mathcal{V})|\psi_E(\vec{x}, \vec{y})\rangle = E|\psi_E(\vec{x}, \vec{y})\rangle
$$

(2)

where

$$
\mathcal{D} = -\frac{T_a}{N_a} \sum_{j=1}^{L} \left[ (\partial_{x_j} - \partial_{x_{j+1}}) \sqrt{x_j x_{j+1}} (\partial_{x_j} - \partial_{x_{j+1}}) \right] \\
- \frac{T_b}{N_b} \sum_{j=1}^{L} \left[ (\partial_{y_j} - \partial_{y_{j+1}}) \sqrt{y_j y_{j+1}} (\partial_{y_j} - \partial_{y_{j+1}}) \right]
$$

is the generalized Laplacian and

$$
\mathcal{V} = -2N_a T_a \sum_{j=1}^{L} \sqrt{x_j x_{j+1}} - 2N_b T_b \sum_{j=1}^{L} \sqrt{y_j y_{j+1}} \\
+ \frac{U_a N_a^2}{2} \sum_{j=1}^{L} x_j (x_j - \epsilon_n) + \frac{U_b N_b^2}{2} \sum_{j=1}^{L} y_j (y_j - \epsilon_m) \\
+W N_a N_b \sum_{j=1}^{L} x_j y_j
$$

(3)

is the generalized potential. The latter provides a remarkably effective way to investigate the ground state structure of Hamiltonian (1) as a function of model parameters. To be more clear, the $2L$-tuples $(\vec{x}, \vec{y})$ which minimize function $\mathcal{V}$ on its domain

$$
\mathcal{R} = \left\{ (x_j, y_j) : 0 \leq x_j, y_j \leq 1, \sum_{j=1}^{L} x_j = \sum_{j=1}^{L} y_j = 1 \right\}
$$

form the ground state structure of the system’s properties far from the thermodynamic limit (in the sense of the statistical-mechanical approach developed in [27]). In Sec. V we present a number of quantum indicators whose critical character corroborates the discussion developed in the previous sections. Eventually, Sec. VI is devoted to concluding remarks.
correspond to those Fock states \(|\tilde{n}, \tilde{m}\rangle\) featuring the largest weights \(c(\tilde{n}, \tilde{m})^2\) in the expansion of the ground state, i.e. in \(|\psi_0\rangle = \sum_{\tilde{n}, \tilde{m}} c(\tilde{n}, \tilde{m})|\tilde{n}, \tilde{m}\rangle\), where the superscript \(Q\) recalls that
\[
Q = \frac{(N_a + L - 1)! (N_b + L - 1)!}{N_a!(L - 1)! N_b!(L - 1)!}
\]
is the dimension of the constant-boson-number subspace contained in the Hilbert space of states associated to Hamiltonian \(\mathcal{H}\).

The determination of the minimum points of potential \(V\) is of particular interest when \(T_a/(U_a N_a) \to 0\) and \(T_b/(U_b N_b) \to 0\). These limiting conditions, in fact, can be regarded as a sort of thermodynamic limit according to the statistical-mechanical approach discussed in \([27]\) and, when they hold, the different phases of the quantum system \(\mathcal{H}\) emerge at their clearest \([18, 19]\). In this limit, generalized potential \(\mathcal{H}\) can be conveniently recast as
\[
V \approx \frac{V}{U_a N_a^2} = \frac{1}{2} \sum_{j=1}^{L} x_j^2 + \frac{\beta^2}{2} \sum_{j=1}^{L} y_j^2 + \alpha \beta \sum_{j=1}^{L} x_j y_j,
\]
an expression which defines a new (rescaled) effective potential which depends only on two effective parameters
\[
\alpha = \frac{W}{\sqrt{U_a U_b}}, \quad \beta = \frac{N_b}{N_a} \frac{\sqrt{U_b}}{\sqrt{U_a}}.
\]
The former constitutes the ratio between the interspecies attractive coupling and the (geometric average of) the intraspecies repulsions, while the latter corresponds to the degree of asymmetry between species \(a\) and species \(b\) condensates. Notice, in particular, that \(\beta \to 1\) in the twin-species scenario, while \(\beta \to 0\) when species \(b\) represents an impurity with respect to species \(a\). In the following, we will assume \(\beta \in [0, 1]\) without loss of generality, as one can always swap species labels in order for \(\beta\) to fall in this interval.

Effective model parameters \(\alpha\) and \(\beta\) have already proved to be the most natural ones to describe the occurrence of rather complex phase-separation phenomena in ultracold binary mixtures loaded in spatially-fragmented geometries \([19]\) and, in the present case, constitute the most effective variables to capture the formation of supermixed solitons. Parameters \(\alpha\) and \(\beta\) span, in fact, a two-dimensional phase diagram where the various phases included therein correspond to different functional dependencies of the minimum-energy configuration \((\tilde{x}_*, \tilde{y}_*)\) and of the relevant energy
\[
V_* := V(\tilde{x}_*, \tilde{y}_*) := \min_{(\tilde{x}, \tilde{y}) \in \mathcal{R}} V(\tilde{x}, \tilde{y})
\]
on \(\alpha\) and \(\beta\) themselves. The presence of different functional dependencies of \(V_*\) on model parameters \(\alpha\) and \(\beta\) results in the presence of borders on the \((\alpha, \beta)\) plane where function \(V_*\) is not analytic, a circumstance which strongly resembles the signature of quantum phase transitions \([29]\).

The search for the configuration \((\tilde{x}_*, \tilde{y}_*)\) which minimizes function \(V\) on its closed domain \(\mathcal{R}\) can be carried out in a fully analytic way. Nevertheless, the complexity of such analysis increases with increasing lattice size \(L\), not only because the interior of region \(\mathcal{R}\) gets bigger and bigger but also (and above all) because the boundary of \(\mathcal{R}\) gets increasingly complex and branched. Indeed, for wide regions of the \((\alpha, \beta)\) plane, it is on the boundary of \(\mathcal{R}\) that \(V_*\) falls, a circumstance which makes it necessary its complete exploration (see \([18]\) for further details on the systematic analysis of the closed \((2L - 2)\)-polytope representing the domain \(\mathcal{R}\)).

III. THE MIXING-SUPERMIXING PHASE DIAGRAM FOR \(T_a/(U_a N_a), T_b/(U_b N_b) \to 0\)

The search for the configuration \((\tilde{x}, \tilde{y})\) minimizing effective potential \(\mathcal{H}\), on its domain \(\mathcal{R}\) has been developed according to the fully-analytic scheme sketched in the previous Sec. and further illustrated in \([18]\). Interestingly, our analysis has highlighted the presence of a common phase diagram for systems featuring \(L = 2\) (dimer), \(L = 3\) (trimer) and \(L = 4\) (tetramer). Such a phase diagram is illustrated in Figure \(\mathcal{I}\) and includes three phases:

i) Phase \(M\) (Mixed) occurs for \(\alpha > -1\) and features uniform boson distribution among the \(L\) wells and mixing of the two species;

ii) Phase PL (Partially Localized), present for \(\alpha < -1\) and \(\beta < -1/\alpha\), is such that the minority species, i.e. species \(b\) (since \(N_b \sqrt{U_b} < N_a \sqrt{U_a}\)), conglomerates and forms a soliton, while the majority species, i.e. species \(a\), occupies all available wells, even if not in a uniform way;

iii) Phase SM (SuperMixed) is marked by the presence of a supermixed soliton (and full localization), meaning that both species conglomerate in the same well.

These three systems therefore feature a common pathway which, upon variation of control parameters \(\alpha\) and \(\beta\), leads from the uniform and mixed configuration (phase \(M\)) to the supermixed soliton (phase \(SM\)), through the intermediate phase (phase \(PL\)), characterized by partial localization, i.e already showing the seed of the soliton, whose emergence, in turn, is due to the localizing effect of the interspecies attraction. For this reason, we conjecture that the mechanism of formation of supermixed solitons is the same regardless of the value of \(L\). To better connote the three presented phases, in Table \(\mathcal{I}\) we give the explicit expressions of \((\tilde{x}_*, \tilde{y}_*)\) as functions of model parameters \(\alpha\) and \(\beta\), together with the relevant value of \(V_*\) (recall relations \(\mathcal{I}\)), in each of the three phases.

We remark that the results listed in Table \(\mathcal{I}\) have been derived in an analytic way (and numerically checked by means of a brute-force minimization of potential \(\mathcal{H}\)) for \(L = 2, 3, 4\) while it is quite natural to conjecture the validity of these results also for \(L \geq 5\). To corroborate
our conjecture, it is worth observing that, for any \( L \),
\( V_\star = V_\star (\alpha, \beta) \) is continuous everywhere in the half-plane \( \{ (\alpha, \beta) : \alpha \leq 0 \text{ and } 0 \leq \beta \leq 1 \} \). In particular, equations
\[
V_\star^M (\alpha = -1, \beta) = V_\star^PL (\alpha = -1, \beta)
\]
and
\[
V_\star^{PL} (\alpha, \beta = -1/\alpha) = V_\star^{SM} (\alpha, \beta = -1/\alpha)
\]
hold, respectively, at phase M-PL and phase PL-SM borders. On the other hand, one can easily realize that the first derivative \( \partial V_\star / \partial \alpha \) is discontinuous at \( \alpha = -1 \) while the second derivative \( \partial^2 V_\star / \partial \alpha^2 \) is discontinuous at \( \beta = -1/\alpha \), regardless of the specific value of \( L \) (see the first panel of Figure 3). This difference in the non-analyticity properties of \( V_\star \) at the two phase boundaries is a direct consequence of the specific functional dependence of \( x_{\alpha,j} \)'s and \( y_{\alpha,j} \)'s on model parameters \( \alpha \) and \( \beta \) in each of the three phases (see second column of Table I). The minimum energy configuration \((\vec{x}_\star, \vec{y}_\star)\), in fact, features a jump discontinuity at transition M-PL while it is continuous at transition PL-SM. In this regard, one can notice that \((\vec{x}_\star, \vec{y}_\star)\) exhibits the same \( Z_L \) symmetry of the trapping potential just in phase M. By making the control parameter \( \alpha \) more negative, one crosses the M-PL border and such symmetry suddenly breaks. A soliton starts to emerge in a certain well, although the remaining \( L - 1 \) wells still include part of the majority species (i.e. species a). Further increasing \( |\alpha| \), the soliton emerges more and more, since all the remaining wells are gradually emptied by the localizing effect of the interspecies attraction. At border PL-SM, the latter has become so strong that both species are fully localized in a certain well, leaving all the remaining ones empty: the supermixed soliton is now completely formed and a further increase of \( |\alpha| \) has no effect on the minimum energy configuration \((\vec{x}_\star, \vec{y}_\star)\). This scenario is pictorially illustrated in Figure 2 for the case \( L = 3 \).

![Phase diagram](image1)

**FIG. 1.** Phase diagram of a bosonic binary mixture featuring attractive interspecies coupling and confined in a generic \( L \)-site potential. Each of the three phases is associated to a specific functional dependence of the minimum-energy configuration \((\vec{x}_\star, \vec{y}_\star)\) and of \( V_\star \) (see relations (7)) on parameters \( \alpha, \beta \). Phase M is the uniform and mixed one, phase PL features a soliton just in the minority species, while phase SM exhibits the presence of a supermixed soliton. Red dashed (solid) line corresponds to a phase transition where the first (second) derivative of \( V_\star \) with respect to \( \alpha \) is discontinuous.

| Phase | \((\vec{x}_\star, \vec{y}_\star)\) | \( V_\star \) |
|-------|---------------------------------|----------------|
| M     | \( x_{\alpha,j} = 1/L \) \( \forall j \) \( y_{\alpha,j} = 1/L \) \( \forall j \) | \( V_\star^M = \frac{1}{2L} (\beta^2 + 2\alpha\beta + 1) \) |
| PL    | \( x_{\alpha,i} = \frac{1 - (L - 1)\alpha\beta}{L} \) \( \forall j \neq i \) \( x_{\alpha,j} = \frac{1 + \alpha\beta}{L} \) \( \forall j \neq i \) \( y_{\alpha,i} = 1, y_{\alpha,j} = 0 \) \( \forall j \neq i \) | \( V_\star^{PL} = \frac{1}{2L} [1 + 2\alpha\beta + \beta^2(L - (L - 1)\alpha^2)] \) |
| SM    | \( x_{\alpha,i} = 1 \) \( x_{\alpha,j} = 0 \) \( \forall j \neq i \) \( y_{\alpha,i} = 1, y_{\alpha,j} = 0 \) \( \forall j \neq i \) | \( V_\star^{SM} = \frac{1}{2} (\beta^2 + 2\alpha\beta + 1) \) |

**TABLE I.** Summary of the different functional dependencies of the minimum-energy configuration and of the relevant value of the effective potential (see relations (7)) in each of the three phases.

![Pictorial representation](image2)

**FIG. 2.** Pictorial representation of the minimum-energy configurations for phases M, PL and SM, in a 3-well system. Vertical axis represent normalized populations \( x_{\alpha,j} \) and \( y_{\alpha,j} \) for the ground state, while numbers 1, 2, 3 label the three wells. The majority (minority) species is depicted in blue (red). In phase M the two species are uniformly distributed in the three wells; in phase PL the minority species forms a soliton while the majority species still occupies all available sites; in phase SM the interspecies attraction is so strong that a supermixed soliton is formed.

**A. Entropy of mixing and Entropy of location as critical indicators**

Two indicators that are well-known in Statistical Thermodynamics and Physical Chemistry [20, 30], the Entropy of mixing and the Entropy of location, can be con-
veniently used to detect the occurrence of phase transitions in the class of systems that we are investigating\[19\]. They are, respectively defined as follows:

$$S_{\text{mix}} = -\frac{1}{2} \sum_{j=1}^{L} \left( x_j \log \frac{x_j}{x_j + y_j} + y_j \log \frac{y_j}{x_j + y_j} \right)$$  \hspace{1cm} (8)

$$S_{\text{loc}} = -\sum_{j=1}^{L} \frac{x_j + y_j}{2} \log \frac{x_j + y_j}{2}.$$  \hspace{1cm} (9)

They provide complementary and somehow orthogonal information about the degree of disorder present in the system. Namely, the former quantifies the degree of mixing while the latter measures the spatial homogeneity of the particles irrespective of their species.

By plugging the expressions of $x_j$, $y_j$’s associated to each of the three phases (see second column of Table 1) into formulas (8) and (9), one can obtain particularly simple expressions for $S_{\text{mix}}$ and $S_{\text{loc}}$ in phase M and in phase SM, which read

$$S_{\text{mix,M}} = \log 2, \quad S_{\text{loc,M}} = \log L,$$

$$S_{\text{mix,SM}} = \log 2, \quad S_{\text{loc,SM}} = 0.$$  

Interestingly, $S_{\text{mix}}$ is the same both in phase M and in phase SM. This indicator, in fact, gives information just about the degree of mixing of the two atomic species, which is indeed the same both in the mixed and in the supermixed phase. Nevertheless, the profound difference between such phases can be appreciated by the combined use of $S_{\text{mix}}$ and $S_{\text{loc}}$, as the latter quantifies the degree of spatial delocalization of the atomic species among the wells. The complete scenario on the $(\alpha, \beta)$-plane is illustrated (for $L = 3$ sites) in the second and in the third panel of Figure 3 where the presence of three qualitatively different regions is evident.

IV. THE DELOCALIZING EFFECT OF TUNNELLING

As already mentioned, the presence of well-recognizable phases in the plane $(\alpha, \beta)$ sharply emerges when $T_a/(U_a N_a) \to 0$ and $T_b/(U_b N_b) \to 0$, two conditions that can be regarded as a sort of thermodynamic limit, according to the statistical-mechanical scheme developed in [27]. Moving away from these limits (either because the numbers of particles $N_a$ and $N_b$ are not large enough or because the hopping amplitudes $T_a$ and $T_b$ have a non-negligible weight in the overall energy balance of the system), the phase diagram illustrated in Figure 1 and discussed in Sec. 3 gets smoothed and deformed, but it is still recognizable. The changes are essentially due to the delocalizing effect of tunnelling terms, which hinder the formation of localized configurations, i.e. of solitons (compare Figures 2 and 4).

In a mathematical perspective, the presence of non-zero tunnelling terms has a regularizing effect on the generalized potential \[3\], whose global minimum can be determined with less effort than in the vanishing-tunnelling case, since such minimum always falls in the \textit{interior} of domain $R$ and never on its \textit{boundary}. One therefore needs to look for the minimum-energy solution of equations $\nabla V = 0$, the gradient being computed with respect to the $2L - 2$ independent variables $x_j$, $y_j$ where $j = 1, 2, \ldots, L - 1$ due to particle-number-conservation constraints.

FIG. 3. Some critical indicators witnessing the presence of three different phases in an $(L = 3)$-site potential (trimer) for $T_a/(U_a N_a) \to 0$ and $T_b/(U_b N_b) \to 0$. First panel: second derivative of functions $V^M_\alpha$, $V^{PL}_\alpha$ and $V^{SM}_\alpha$ (see third column of Table 1) with respect to control parameter $\alpha$ for $L = 3$. One can appreciate that it is discontinuous both at border PL-SM and at border M-PL (in the latter border the first derivative $\partial V_\alpha/\partial \alpha$ is already discontinuous). Second and third panel: critical indicators $S_{\text{mix}}$ and $S_{\text{loc}}$ associated to the minimum-energy configuration $(x^*, y^*)$ (obtained, in turn, setting $L = 3$ in the second column of Table 1).
We have fully developed this analysis for $L = 2$ (dimer), $L = 3$ (trimer) and $L = 4$ (tetramer). Although we refer to Figure 5 (obtained setting $L = 3$) for the sake of clarity, the following observations have been proved to hold for $L = 2, 3, 4$ and are conjectured to be still valid also for $L \geq 5$:

- Contrary to the zero-tunneling case, critical indicators $S_{\text{mix}}$ and $S_{\text{loc}}$ are continuous functions of model parameters $\alpha$ and $\beta$. This circumstance is due to the fact that normalized boson populations $x_j$’s and $y_j$’s themselves no longer feature jump discontinuities. Nevertheless, both indicators are still able to witness the presence of three qualitatively different regions in the $(\alpha, \beta)$ plane.

- Supported by tunneling processes, the mixed phase survives beyond the border $\alpha = -1$, provided that $\beta = N_b \sqrt{U_b} / (N_a \sqrt{U_a})$ is small enough. In this case, in fact, the interspecies attraction is hindered by the delocalizing effect of $T_a$ and $T_b$ so much that it is unable to trigger soliton formation. Interestingly, by resorting to the Hessian matrix associated to effective potential [3], it is possible to derive inequality

$$\alpha > -\sqrt{\left(1 + \frac{9}{2} \frac{T_a}{U_a N_a}\right) \left(1 + \frac{9}{2} \frac{T_b}{U_b N_b}\right)} \quad \text{(10)}$$

giving the region of parameters’ space where the uniform configuration $x_j = y_j = 1/3$ is the least energetic one. This region, whose border is depicted with dashed lines in Figure 5, coincides (in the limit $N_a = N_b$, $T_a = T_b$, $U_a = U_b$) with the portion of parameters' space where Bogoliubov quasi-particle frequencies are well defined [31] (we remark that such spectrum was computed assuming the macroscopic occupation of a momentum mode).

- The formation of a supermixed soliton, the configuration for which $S_{\text{loc}} = \log L$, is only slightly hindered by the presence of tunneling processes. The latter tend to delocalize the atomic species among the wells and are responsible for the survival of non-zero tails in wells far from the supermixed soliton. Nevertheless, such tails, which are fully reabsorbed by the soliton only in the limit $\alpha \to -\infty$, do not significantly affect the solitonic structure of the minimum-energy configuration (see third panel of Figure 4). This circumstance is witnessed by the fact that, in the upper left part of the phase diagram, $S_{\text{loc}}$ is only slightly lower than $\log L$ (see second panel of Figure 5).

With reference to Figure 5, we remark that, along the dashed lines (representing the border between phase M and phase PL and given by formula (10)), the Bogoliubov frequencies computed assuming the macroscopic occupation of a momentum mode vanish [31]. Conversely, along the solid lines (representing the border between phase PL and phase SM and given by formula (23)), the Bogoliubov frequencies computed assuming the macroscopic occupation of a site mode vanish (see Appendix A).
A. Uniform configuration for a generic \( L \)-site potential

It is possible to analytically derive the counterpart of inequality (10), which holds for \( L = 3 \), both for the dimer (\( L = 2 \)) and for the tetramer (\( L = 4 \)). These inequalities, ensuing from the condition that the Hessian matrix associated to generalized potential \( \mathcal{E} \) and evaluated at point \( x_j = y_j = 1/L \) is positive definite, respectively read

\[
\alpha > -\sqrt{\left(1 + 2 \frac{T_a}{U_a N_a}\right) \left(1 + 2 \frac{T_b}{U_b N_b}\right)} \tag{11} \]

and

\[
\alpha > -\sqrt{\left(1 + 4 \frac{T_a}{U_a N_a}\right) \left(1 + 4 \frac{T_b}{U_b N_b}\right)} \tag{12} \]

It is worth mentioning that their twin-species limits (i.e. their expression when \( N_a \to N_b, U_a \to U_b \) and \( T_a \to T_b \)) coincide with the inequalities giving the regions of parameters’ space where Bogoliubov quasi-particle frequencies are well defined. The latter have been derived, assuming the macroscopic occupation of a momentum mode, for the dimer in \([28]\) and in \([31]\), thanks to the dynamical algebra method, for a ring lattice. In view of these results and of the rather general formulas giving the condition for the collapse of Bogoliubov frequencies in a generic (\( L \geq 3 \))-site ring lattice (see \([31]\)), it is quite natural to conjecture that, for a generic \( L \)-site potential and for \( T_a \neq T_b, U_a \neq U_b \) and \( N_a \neq N_b \), inequality

\[
\alpha > -\sqrt{\left[1 + C_L \frac{T_a L}{U_a N_a}\right] \left[1 + C_L \frac{T_b L}{U_b N_b}\right]} \tag{13} \]

where \( C_L = 1 - \cos(2\pi/L) \), gives the region of parameters’ space where the uniform solution \( x_j = y_j = 1/L \) is the least energetic one. Remarkably, in the limit \( T_a/(U_a N_a) \to 0 \) and \( T_b/(U_b N_b) \to 0 \), inequalities (10), (11), (12) and (13) reduce to \( \alpha > -1 \), the condition which was shown to constitute the border between phase M and PL in the thermodynamic limit (see Figure 1). In passing, one can observe that, for \( L = 2 \), the mismatch between inequalities (13) and (11) is only apparent, in that the former is referred to a system inherently featuring the ring geometry which is absent in the dimer.

V. QUANTUM CRITICAL INDICATORS

The mechanism of formation of supermixed solitons presented in Sec. III and IV by means of a semiclassical approach capable of highlighting, in a rather transparent way, the presence of three different phases in the plane \((\alpha, \beta)\), is fully confirmed by genuinely quantum indicators. To develop the quantum analysis, one has to perform the exact numerical diagonalization of Hamiltonian \( H \) in order to determine the ground state

\[
|\psi_0\rangle = \sum_{\vec{n}, \vec{m}} c(\vec{n}, \vec{m}) |\vec{n}, \vec{m}\rangle \tag{14} \]

the associated energy

\[
E_0 = \langle \psi_0 | H | \psi_0 \rangle \tag{15} \]

and the first excited levels

\[
E_i = \langle \psi_i | H | \psi_i \rangle \tag{16} \]

Of particular importance for the current investigation are coefficients \( c(\vec{n}, \vec{m}) \) appearing in expansion (14) and defined as

\[
c(\vec{n}, \vec{m}) = \langle \vec{n}, \vec{m} | \psi_0 \rangle \tag{17} \]

which will be used to introduce the quantum counterparts of indicators (3) and (9). The diagonalization of Hamiltonian (1) is carried out for extended sets of model parameters, in such a way to explore vast regions of the \((\alpha, \beta)\)-plane (recall formulas (6)), also in relation with the presence of non-negligible hoppings \( T_a \) and \( T_b \). This analysis allows one to appreciate the dependence of some genuinely quantum indicators on model parameters and, above all, their being critical along the same curves of the \((\alpha, \beta)\)-plane where the semiclassical approach predicts the occurrence of mixing-supermixing transitions. For the sake of clarity, we will refer to Figure 6, whose rows correspond to different quantum indicators and whose columns to different values of the hopping amplitude \( T := T_a = T_b \). Going from left to right, it reads

\[
T = 0.2, 0.5, 0.8 \tag{18} \]

respectively. In general, the same observations that we made in Sec. VII concerning the delocalizing effect of tunnelling and the impact thereof on \( S_{\text{mix}} \) and on \( S_{\text{loc}} \) hold also within this purely quantum scenario. In particular, one can notice that: i) All quantum indicators are continuous functions of model parameters \( \alpha \) and \( \beta \); ii) The mixed phase is supported by tunnelling processes, iii) The formation of supermixed solitons occurs for large values of \( |\alpha| \) and moderate values of \( \beta \).

The quantum critical indicators which have been scrutinized in relation to the mixing-supermixing transitions are the following:

**Ground-state energy.** Indicator (15), regarded as a function of effective model parameters \( \alpha \) and \( \beta \) can effectively witness the presence of three different phases (corresponding to the already discussed phase M, phase PL and phase SM). To be more clear, function \( E_0(\alpha, \beta) \) is everywhere continuous in the \((\alpha, \beta)\)-plane, but it features non analiticities, either in its first or in its second derivative, along two specific lines of the phase diagram which, in turn, divide the latter into three separate regions. The functional dependence of \( E_0 \) in each of the three regions
is different, that means that the slope $\partial E_0/\partial \alpha$ and the concavity $\partial^2 E_0/\partial \alpha^2$ exhibit different behaviours.

This circumstance is well illustrated in the first row of Figure 6, where we have plotted $\partial^2 E_0/\partial \alpha^2$ (the logarithmic scale has been adopted just for graphical purposes) for three different values of the hopping amplitude. The left panel, obtained for $T/U_a = 0.2$, allows one to recognize two regions (in green), well separated by an intermediate region (in red-orange) which intercalates between them. In the central and in the right panels, which feature bigger hopping amplitudes ($T/U_a = 0.5$ and 0.8 respectively), the presence of the intermediate phase (phase PL) is still evident, although it turns out to be slightly deformed and its borders less sharp.

Entropy of mixing. In Sec. III we introduced indicator (8) and discussed its ability to quantify the degree of mixing of a semiclassical configuration $(\vec{x}, \vec{y})$. A reasonable quantum mechanical version of this indicator can be constructed as follows: after determining the complete decomposition (14) of the system’s ground state $|\psi_0\rangle$ and, in particular, the full list of coefficients (17) (the cardinality of this set being given by formula (9)), one can evaluate the entropy of mixing of $|\psi_0\rangle$ by defining

$$S_{mix} := \sum_{\vec{n}, \vec{m}} |c(\vec{n}, \vec{m})|^2 S_{mix}(\vec{n}, \vec{m}),$$

where $S_{mix}(\vec{n}, \vec{m})$ is the entropy of mixing of the state $|\psi_0\rangle$ of the Fock basis, computed by means of formula (8) (with the obvious identifications $x_j = n_j/N_a$ and $y_j = m_j/N_b$).

The indicator thus obtained is illustrated, as a function of model parameters $\alpha$ and $\beta$, in the second row of Figure 6 for the three choices (18). Especially for small hoppings, one can observe the presence of an intermediate phase (phase PL) which stands in between phase SM and phase M. Increasing the tunnelling, the intermediate phase (phase PL) which stands in between phase M and phase PL takes place, a circumstance which has been already noticed in relation to mixing-demixing transitions [17, 18, 21]. Among various possibilities, we have focused on the entropy of entanglement between species a and species b. As a consequence, the entanglement between the two atomic species is given by

$$EE = -\text{Tr}_a(\hat{\rho}_a \log_2 \hat{\rho}_a),$$

an expression corresponding to the Von Neumann entropy of the reduced density matrix

$$\hat{\rho}_a = \text{Tr}_b(\hat{\rho}_0).$$

The latter can be obtained, in turn, by tracing out the degrees of freedom of species b from the ground state $|\psi_0\rangle$, which, in turn, can radically change upon variation of model parameters [17, 18, 21]. Further increasing $|\alpha|$, a plateau is reached, wherein the $EE$ stabilizes to the limiting value of $\log L = \log 3 \approx 1.59$. The argument of the logarithm (which is set to $L = 3$ in the example shown in Figure 6), corresponds to the number of semiclassical configurations minimizing potential (7) and which are quantum-mechanically reabsorbed in the formation of a unique non-degenerate ground state. In other words, the $L$-fold degeneracy of the semiclassical configuration corresponding to the presence of a supermixed soliton in one of the $L$ wells is lifted by the presence of tunnelling, which therefore determines the formation of a $L$-faced Schrödinger cat.

Energy spectrum. The computation of the first excited energy levels of the system (see formula (16)) as a function of control parameter $\alpha$ can give an additional physical insight and a further confirmation of the presence of...
three qualitatively different phases. Figure 7 illustrates the energy fingerprint of a $L = 3$ system, for $\beta = 0.6$ and the usual values (18). With reference to the left panel, the one featuring the smallest value of $T/U_a$, it is possible to distinguish three different regions wherein the energy-levels arrangement is qualitatively different. For small values of $|\alpha|$, the levels can be shown to well match Bogoliubov’s quasi-particles frequencies which are, in turn, computed assuming the macroscopic occupation of momentum mode $k = 0$ (see [31]). At $\alpha \approx -1$ all these levels collapse, thus signing the end of phase M and, further increasing $|\alpha|$ they manifestly rearrange (it is worth mentioning that, for $\alpha < -1$ some excited levels seem to coincide with the lowest one, but, actually, this overlap is just apparent and merely due to the scale used for the vertical axis). Further increasing $|\alpha|$ down to $\alpha \approx -1.7$, another qualitative change of the energy levels’ structure is met, which constitutes the border between phase PL and phase SM. At such value of $\alpha$, in fact, the energy levels, although they do not collapse, assume a distinctly-linear functional dependence on $\alpha$. The presence of three regions where the energy fingerprint is qualitatively different can be noticed also in the central and in the right panel of Figure 7, although the critical behaviours (namely the spectral collapse and the onset of the linear ramp) are smoothed down by the delocalizing effect of tunnelling. In this regard, one can observe that tunnelling is responsible also for the leftward translation of the collapse point (see formula (10) and the discussion thereof).

FIG. 6. Each row illustrates the behaviour of a genuinely quantum indicator as a function of model parameters $\alpha$ and $\beta$. Each column corresponds to a different value of the ratio $T/U_a$, where $T := T_a = T_b$ (from left to right, $T/U_a = 0.2$, $0.5$, $0.8$). First row: second derivative of the ground-state energy $E_0$ (see formula 15) with respect to $\alpha$. The logarithmic scale is used in order to better visualize the presence of three qualitatively different regions. Second row: quantum version of the entropy of mixing, $\tilde{S}_{\text{mix}}$ (see formula 19). Third row: quantum version of the entropy of location $\tilde{S}_{\text{loc}}$ (see formula 20). Fourth row: entanglement between the two condensed species, $EE$ (see formula (21)). Model parameters $L = 3$, $N_a = N_b = 15$, $U_a = 1$, $U_b \in [0,1]$ and $W \in [-3,0]$ have been used.

VI. CONCLUDING REMARKS

In this work, we have investigated the mechanism of soliton formation in bosonic binary mixtures loaded in ring-lattice potentials. Our analysis has evidenced that all these systems, irrespective of the number sites, share...
a common mixing-demixing phase diagram. The latter is
spanned by two effective parameters, $\alpha$ and $\beta$, the first
one representing the ratio between the interspecies attrac-
tion and the (geometric average of) the intraspecies repulsions, the second one accounting for the degree of
asymmetry between the species. Such phase diagram
includes three different regions, differing in the degree of
mixing and localization. The first phase, occurring for
sufficiently small $|\alpha|$, is the mixed one (phase M) and
it is such that the atomic species are perfectly mixed
and uniformly distributed among the wells. The second
phase (phase PL) occurs for moderate values of $|\alpha|$ and
sufficiently asymmetric species. It includes the local-
ized soliton-like states, although the latter are not de-
veloped in a full way. Eventually, the third phase (phase
SM), occurring for sufficiently large values of $|\alpha|$, corre-
sponds to states such that both atomic species clot in the
same unique well, hence the name supermixed solitons.

After introducing the quantum model and its represen-
tation in the CVP, in Sec. [IV] the mixing-supermixing
transitions are derived within such semiclassical approxi-
mation scheme which transparently shows the emergence
of a bi-dimensional phase diagram. The three phases
therein not only feature specific functional dependences
of the ground-state energy on model parameters, but also
are characterized in terms of two critical indicators im-
ported from Statistical Thermodynamics, the entropy of
mixing and the entropy of location.

Sec. [V] is devoted to the analysis of finite size effects,
i.e. how the phase diagram changes and gets blurred if one
walks away from the thermodynamic limit (in the sense
specified within the statistical mechanical approach
developed in [27]). The delocalizing effect of tunneling is
shown to favor the mixed phase and to hinder the for-
mation of solitons but not to upset the presented phase
diagram. Quantum indicators are presented in Sec. [V]
whose critical behaviour along certain lines of the phase
diagram $(\alpha, \beta)$ corroborates the scenario that emerged
from the semiclassical treatment of the problem.

In conclusion, we note that the methodology on which
our analysis relies, together with the classical and quan-
tum indicators used to detect critical phenomena, can
be easily applied to systems with more complex lattice
topologies and tunnelling processes [32] [35]. In view of
this, and considering the increasing interest for multicom-
ponent condensates [30] [39], our future work will aim to
extend the presented analysis to the soliton formation’s
mechanism in complex lattices and in presence of mul-
tiple condensed species.

Appendix A

In this appendix, we derive, by means of a modified
version of the Bogoliubov approximation scheme [31] [40],
the analytical expression of quasiparticles’ frequencies
of a $L = 3$-system when its ground state exhibits a super-
mixed soliton-like structure (namely, when it belongs to
phase SM). In this circumstance, in fact, one can rec-
ognize that there are two site modes, $a_1$, $b_1$, that are
macroscopically occupied, namely $n_1 \approx N_a - n_2 - n_3$ and
$n_1 \approx N_b - m_2 - m_3$ while the microscopically occupied
ones are $a_2$, $a_3$, $b_2$ and $b_3$. With these substitutions in
mind, one can derive $H^{(2)}$, the quadratic approxima-
tion of the original Hamiltonian $H^{(0)}$, which reads

$$H^{(2)} = -T_a (a_3^\dagger a_2 + a_2^\dagger a_3) - (U_a N_a + N_b W)(n_2 + n_3)$$

$$- T_b (b_3^\dagger b_2 + b_2^\dagger b_3) - (U_b N_b + N_a W)(m_2 + m_3).$$

Notice that we have neglected not only higher-order terms but also linear terms, since the latter contribute just to the ground-state energy but do not affect the characteristic frequencies and, in general, they can be removed by a suitable unitary transformation.

Recognizing that terms

$$J_+ = a_2 a_3^\dagger, \quad J_- = a_2^\dagger a_3, \quad J_3 = \frac{1}{2}(n_3 - n_2)$$

constitute the two-boson realization of algebra su(2), one
can easily diagonalize $H^{(2)}$ enacting the unitary transforma-
tion $U_\varphi = e^{\frac{i}{2}(J_+ - J_-)}$ which gives

$$U_\varphi (J_+ + J_-) U_\varphi^\dagger = 2J_3 \sin \varphi + (J_+ + J_-) \cos \varphi.$$

Treating in the same way terms $b_j$’s, it is straightforward
to derive diagonal Hamiltonian

$$H_D = n_2 (T_a - U_a N_a - N_b W) + n_3 (-T_a - U_a N_a - N_b W)$$

$$+ m_2 (T_b - U_b N_b - N_a W) + m_3 (-T_b - U_b N_b - N_a W),$$

an expression where the coefficients of number oper-
ators constitute the Bogoliubov quasiparticles’ frequen-
cies, namely $H_D = \omega_3 n_2 + \omega_3 n_3 + \Omega_2 m_2 + \Omega_3 m_3$. As
illustrated in Figure [8] the agreement between the spec-
trum envisaged by this approximation scheme and the ex-
act one, obtained numerically, is good, not only qualita-
atively (same linear behaviour) but also quantitatively
(<10% of difference if $|\alpha|$ is large enough). This agree-
ment rapidly improves as soon as the numbers of particles
$N_a$ and $N_b$ increase.
Interestingly, the simultaneous validity of conditions
\[ \omega_2 > 0, \quad \omega_3 > 0, \quad \Omega_2 > 0, \quad \Omega_3 > 0 \] (23)
gives the region of parameters' space where Hamiltonian \( H_D \) is lower bounded, i.e., the region where the supermixed soliton-like configuration is estimated to be stable. The border of this region corresponds to the solid lines present in Figure 5 which, in turn, stand where indicators \( S_{mix} \) and \( S_{loc} \) illustrated therein feature criticalities.

In conclusion, we remark that the approximation scheme developed in this appendix is based on the assumption of macroscopic occupation of site modes (one for each component) and that it is able to estimate the energy spectrum for large values of \( |\alpha| \), i.e., in phase SM. This scheme is therefore fundamentally different from the one developed in [31] and linked to condition (10), since the latter was based on the assumption of macroscopic occupation of momentum mode \( k = 0 \) and was therefore intended to approximate the energy spectrum for small values of \( |\alpha| \) (a circumstance corresponding, in turn, to uniform boson configuration, i.e., to phase M).

![FIG. 8. Red lines: first excited levels of the exact spectrum obtained by means of numerical diagonalization of Hamiltonian \( \hat{H} \). Blue lines: Bogoliubov characteristic frequencies present in diagonal Hamiltonian \( H_D \). The following model parameters have been chosen: \( L = 3, T_a = T_b = 0.2, U_a = 1, U_b = 0.36, N_a = N_b = 15, W \in [-1.8, 0] \).](image)

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