Droplet under confinement: Competition and coexistence with soliton bound state

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We study the stability of quantum droplet and its associated phase transitions in ultracold Bose-Bose mixtures uniformly confined in quasi-two-dimension. We show that the confinement-induced boundary effect can be significant when increasing the atom number or reducing the confinement length, which destabilizes the quantum droplet towards the formation of a soliton bound state. In particular, as increasing the atom number we find the reentrance of soliton ground state, while the droplet is stabilized only within a finite number window that sensitively depends on the confinement length. Near the droplet-soliton transitions, they can coexist with each other as two local minima in the energy landscape. Take the two-species$^{39}$K bosons for instance, we have mapped out the phase diagram for droplet-soliton transition and coexistence in terms of atom number and confinement length. The revealed intriguing competition between quantum droplet and soliton under confinement can be readily probed in current cold atoms experiments.

\textit{Introduction.} Quantum droplet describes a self-bound many-body state that is stabilized by quantum effect. It has intrigued great attention recently in the field of ultracold atoms, given its successful observation in dipolar gases\cite{1–7} and alkali Bose-Bose mixtures\cite{8–11}. These dilute droplets, as pointed out in a pioneer work by Petrov\cite{12}, are stabilized by a subtle balance between the mean-field attraction and the Lee-Huang-Yang(LHY) repulsion from quantum fluctuations. Similar stabilization mechanism has been extended to other droplet systems including Bose-Fermi mixtures\cite{13–18} and dipolar mixtures\cite{19, 20}.

The stability of quantum droplet depends crucially on the geometry. In three-dimension(3D), the quantum pressure can dissociate the droplet at small atom number and lead to the liquid-gas transition as observed in experiments\cite{1–11}. In 2D and 1D, quantum droplet can be supported in quite different interaction regimes as compared to 3D, due to distinct LHY corrections\cite{21}. In this context, it is conceptually important and also practically meaningful to investigate the confinement effect to droplet stability, which can bridge different droplet physics between different geometries. Previously, a few theoretical studies have revealed the significant change of LHY correction in quasi-low dimensions\cite{22–25}. In particular, it has been shown that for alkali bosons the LHY energy can gradually change sign to negative as deepening the confinement\cite{24, 25}, while the resulted instability of droplet and its associated transitions during the dimensional reduction have not been discussed therein.

Apart from the significant change of LHY correction, the confinement will affect the droplet stability in two other non-trivial ways:

First, it introduces the boundary effect. As illustrated in Fig.1, for a droplet cloud confined uniformly with well-defined boundaries(central plot), the boundary effect can become significant when the droplet size $\sigma$ is comparable to the trap length $L$, either by increasing atom number $N$(right) or by reducing $L$(left). In either case, the droplet will adjust itself to be compatible with the boundary, which naturally causes instability. Second, the confinement can introduce another channel of bound state to compete with the droplet. A well known example is the bright soliton in quasi-1D(q1D) that is stabilized by quantum pressure and mean-field attraction\cite{26–28}. In a recent experiment of Bose-Bose mixture\cite{9}, the droplet-soliton transition was explored in harmonically trapped quasi-1D, while the confinement effect to qualitative change of LHY correction was not considered.

In this work, by fully taking into account the confinement effect, we study the stability of quantum droplet and its associated transitions in Bose-Bose mixtures confined in q2D. To clearly see the boundary effect, we take the uniform confinement as depicted in Fig.1, which has become experimentally accessible with a tunable length\cite{29–33}. We find that when the boundary effect becomes significant, as schematically shown in Fig.1, the
droplet will become unstable and give way to a soliton bound state that displays no density modulation along the confined direction. This leads to the reentrance of soliton ground state as increasing atom number, while the droplet can be stabilized only within certain number window that sensitively depends on the trap near. Under droplet-soliton transitions, they can coexist with each other as two local minima in the energy landscape. Take the $^{39}$K Bose-Bose mixture for example, we have analyzed in detail the competition physics between droplet and soliton and further mapped out the phase diagram for their transition and coexistence in terms of atom number and confinement length. These results can be readily tested in current cold atoms experiments.

**Model.** We consider the Hamiltonian for the Bose-Bose atomic mixture $H = \int dr H(r)$ with: ($\hbar = 1$)

$$H(r) = \sum_{i=1,2} \Psi_i^\dagger(r) \left(-\frac{\nabla^2}{2m_i}\right) \Psi_i(r) + \sum_{ij} \frac{g_{ij}}{2} \Psi_i^\dagger \Psi_j \Psi_j \Psi_i(r).$$

Here $r = (x, y, z)$ is the coordinate; $m_i$ and $\Psi_i$ are respectively the mass and field operator of boson species $i$: $g_i = 4\pi a_{i1}/m_i$ and $g_{12} = 2\pi a_{12}/(\mu = m_1 m_2/(m_1 + m_2))$ are the intra- and inter-species coupling constants. Given the atoms confined in a uniform trap with $z \in [-L, L]$ and under periodic boundary condition, the momentum along the intra- and inter-species coupling constants. Given the atoms confined in a uniform trap with $z \in [-L, L]$ and under periodic boundary condition, the momentum along the confined direction. This leads to the reentrance of soliton ground state as increasing atom number, while the droplet can be stabilized only within certain number window that sensitively depends on the trap near. Under droplet-soliton transitions, they can coexist with each other as two local minima in the energy landscape. Take the $^{39}$K Bose-Bose mixture for example, we have analyzed in detail the competition physics between droplet and soliton and further mapped out the phase diagram for their transition and coexistence in terms of atom number and confinement length. These results can be readily tested in current cold atoms experiments.

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**Results.** For searching for the energy minimum in terms of $\sigma_{xy}$ and $\sigma_z$, we consider the two hyperfine states of $^{39}$K atoms, $|1\rangle \equiv |F = 1, m_F = 0\rangle$, $|2\rangle \equiv |F = 1, m_F = -1\rangle$, as have been well studied in 3D droplet experiments[8–10]. In this case, $a_{22} = 35a_B$, $a_{12} = -53a_B$ ($a_B$ is the Bohr radius), and $a_{11}$ is highly tunable by magnetic field. We will focus on the mean-field collapse regime with $\delta a \equiv a_{12} + \sqrt{a_{11} a_{22}} < 0$ and study how the uniform confinement affects the quantum droplet. As we consider small $|\delta a| \ll |a_{11}, a_{22}|$, in calculating $E_{\text{LHY}}$ we make the approximation $\delta a = 0$ to avoid the photon instability due to complex spectrum (2). Other rectified theories on this have appeared recently[35–37]. Throughout the paper, we choose the length unit as $l_0 = 1 \mu m$ of the energy unit as $E_0 = 1/(2ml_0^2)$, with mass $m \equiv m_1 = m_2$ for $^{39}$K atoms.

**Droplet solution.** Fig.2 shows the droplet solution as varying $N$ at several typical $L$. One can see from Fig.2(a) that the droplet energy continuously decreases as shrinking $L$, which can be attributed to the reduced kinetic and LHY energies. Moreover, another remarkable effect of finite $L$ is that, now the droplet only survives within a finite number window $[N_{d1}, N_{d2}]$, unlike the free space droplet that just requires a lower number bound. This number window becomes narrower for smaller $L$, due to the existence of another competitive channel of bound state (soliton, as discussed later). In particular, we see that a small $L$ also gives rise to a small upper bound $N_{d2}$, and this is consistent with the boundary effect as illustrated in Fig.1.

Fig.2(b1,b2) show that the droplet sizes $\sigma_{xy}$ and $\sigma_z$ both evolve non-monotonically with $N$. Near the vanishing point of droplet ($N \sim N_{d2}$), shrinking $L$ will lead to a smaller $\sigma_{xy}$ but a larger $\sigma_z$. This means that by tight-
enishing the confinement, more weight of the droplet transfers from the free (xy) to confined (z) direction; accordingly, its wave function will change from a nearly isotropic shape (3D case) to a highly elongated one (more extended along z), as shown in Fig. 2(c). This counter-intuitive change can be understood as follows: a tight confinement (small \( L \)) can induce a large energy gap along \( z \), and therefore the system tends to minimize the density modulation in this direction to suppress \( E_{\text{kin}} \), which leads to a more extended wave function along \( z \).

\[ \sigma_{2D} = 4LD^{1/2}\exp\left(\frac{1}{2} - \frac{NC}{4D^2}\right), \]

\[ \sigma_{3D} = \frac{1024L D^{5/2}}{25\pi^2 NC^2}, \]

for \( C = -1 - 2N_1 N_2 \delta a/(NL) \) and \( D = (N_1 a_1 + N_2 a_2)/(2L) \). In Fig. 3 we show the soliton size \( \sigma_{xy} \) as varying \( N \) at fixed \( L = 3 \mu m \), and we see that Eqs. (5,6) fit well to \( \sigma_{xy} \) respectively in small and large \( N \) limit.

\( \text{(III) Droplet-soliton transition and coexistence.} \) After identifying the individual property of droplet and soliton, now we turn to investigate their competition. In Fig. 4, we demonstrate their transition and coexistence as tuning \( N \) for a fixed \( L = 3.5 \mu m \). As seen from Fig. 4(a), the energies of droplet and soliton cross twice as increasing \( N \), which determine two transition points respectively at \( N_{c1} \) and \( N_{c2} \). Their individual stability and mutual competition can be clearly seen from the energy contour plots \( E(\sigma_{xy}, \sigma_z) \) in Fig. 4(c1-c5), together with the comparison of their transverse sizes \( \sigma_{xy} \) shown in Fig. 4(b).

For small \( N \), the only energy minimum represents a soliton state, i.e., at \( \sigma_z \to \infty \) and a finite \( \sigma_{xy} \) (see Fig. 4(c1)). As increasing \( N \) to \( N_{d1} \), the droplet start to emerge as an additional energy minimum at finite \( \sigma_z \) and a smaller \( \sigma_{xy} \) (see Fig. 4(b)). The double minima reach the same energy when tune \( N \) to the first transition point \( N_{c1} \) (see Fig. 4(c2)).

To facilitate the discussion, let us define the droplet region in the energy landscape along \( \sigma_{xy} \), with lower bound \( \sigma_{xy}^{d,\text{low}} \) and upper bound \( \sigma_{xy}^{d,\text{upp}} \) (marked by the dashed dot and dashed lines in Fig. 4(c2-c4)). Within this region, i.e., for any \( \sigma_{xy} \in (\sigma_{xy}^{d,\text{low}}, \sigma_{xy}^{d,\text{upp}}) \), the energy minimum occurs at a finite \( \sigma_z \). Once the soliton enters this region, i.e., when its size \( \sigma_{xy} \in (\sigma_{xy}^{s,\text{low}}, \sigma_{xy}^{s,\text{upp}}) \), the soliton will become unstable and flow from \( \sigma_z = \infty \) to the droplet minimum. In Fig. 4(b), we denote the atom number at the intersection of \( \sigma_{xy}^{s} \) and \( \sigma_{xy}^{d,\text{upp}} \) (\( \sigma_{xy}^{d,\text{low}} \)) as \( N_{s1} (N_{s2}) \). Correspondingly, when \( N \in [N_{s1}, N_{s2}] \), the soliton becomes locally unstable and the droplet is the only stable (ground) state, see Fig. 4(c3). For \( N \) beyond \( N_{s2} \), the soli-
sizes along free \( z \) direction, or equivalently, when they have similar discontinuous number change or droplet fragmentation, and their transitions can be explored through the density modulations along the confined direction, and thus the soliton state is always more favored for any particle number.

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Their phase boundaries are given by \( N_{d1}, N_{c1}, N_{c2} \) and \( N_{d2} \) (see text). Droplet-soliton transitions (energy crossing) occur at \( N_{c1} \) and \( N_{c2} \), denoted by solid and hollow orange diamonds.

\[ \sigma_z = 1.86 \mu \text{m}, \text{beyond half of trap length } L = 3.5 \mu \text{m}. \]

\[ \delta a = -5 a_B. \] The droplet, soliton, and their coexistence regions are respectively shown by blue, white, and gray colors. Their phase boundaries are given by \( N_{d1}, N_{c1}, N_{c2} \) and \( N_{d2} \) (see text). Droplet-soliton transitions (energy crossing) occur at \( N_{c1} \) and \( N_{c2} \), denoted by solid and hollow orange diamonds.

\( \text{(IV) Phase diagram.} \) To fully explore the confinement effect, we have carried out similar analysis for different \( L \) and arrived at the phase diagram in the \( (N, L) \) plane as shown in Fig.5. One can see that the droplet state (blue color) only survives within a finite number window that sensitively depends on the value of \( L \). It will give way to the soliton state (white color) for very large or small \( N \), or for small \( L \). Near their transition points \( N_{c1} \) and \( N_{c2} \) (orange diamonds), the droplet and soliton can coexist with each other, and their coexistence region (gray color) also depends sensitively on \( L \).

In fact, for \( L \in (2.6, 3) \mu \text{m} \) we find continuous transitions between droplet and soliton, i.e., the location of energy minimum continuously change between finite and infinite \( \sigma_z \) across the phase boundaries; for \( L < 2.6 \mu \text{m} \), no droplet solution can be found and the soliton is the only stable (ground) state. A physical picture for this finding is that, for very small \( L \), the large energy gap along \( z \) rules out the possibility of density modulation in this direction, and thus the soliton state is always more favored for any particle number. Fig.5 can be readily detected in experiments. The droplet and soliton states can be identified by measuring their density modulations along the confined direction, and their transitions can be explored through the discontinuous number change or droplet fragmentation when sweeping across the phase boundary, as recently conducted in experiment with a different setup[9].
Discussion. In this work we have adopted the local density approximation (LDA) to compute $E_{\text{LHY}}$, which was shown to predict the transitions in 3D droplets quantitatively well\cite{8, 10}. Here we remark that the LDA is even more qualified in our case, especially along the confined direction with small $L$. This is because as reducing $L$, the droplet density gets more elongated along $z$ (see Fig. 2(c)) and the kinetic energy is further suppressed. In fact, we have checked that $\eta_z \equiv E_{\text{kin},z}/E_{\text{LHY}} \ll 1$ is satisfied in a broad parameter regime we considered. Take the case in Fig. 4 for instance, the ratio $\eta_z$ is 0.46 at $N_{c1}$ and gets even smaller to 0.08 at $N_{c2}$. This is to say, the typical length at which the density varies is visibly longer than that characterizing the LHY correction, which justifies the application of LDA in our setup.

Finally, it is worth to point out that the boundary effect revealed here is unlikely to apply for harmonic confinements, where the boundary cannot be clearly defined. This expectation is consistent with the recent experimental study of harmonically trapped Bose-Bose mixtures in q1D, where only one droplet-soliton transition (corresponding to $N_{c1}$ in this work) was observed\cite{9}.

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