Lee-Huang-Yang effects in the ultracold mixture of $^{23}$Na and $^{87}$Rb with attractive interspecies interactions

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The beyond-mean-field Lee-Huang-Yang (LHY) correction is ubiquitous in dilute ultracold quantum gases. However, its effects are often elusive due to the typically much larger influence of the mean-field energy. In this work, we study an ultracold mixture of $^{23}$Na and $^{87}$Rb with tunable attractive interspecies interactions. The LHY effects manifest in the formation of self-bound quantum liquid droplets and the expansion dynamics of the gas-phase sample. A liquid-to-gas phase diagram is obtained by measuring the critical atom numbers below which the self-bound behavior disappears. In stark contrast to trapped gas-phase condensates, the gas-phase mixture formed following the liquid-to-gas phase transition shows an anomalous expansion featuring a larger release energy for increasing mean-field attractions.

Bose-Einstein condensate (BEC) of dilute atomic gases is a very natural platform for testing the rich physics of interacting Bose gases. While the behavior of BECs is typically dictated by the mean-field (MF) interaction, effects caused by the beyond-mean-field Lee-Huang-Yang (LHY) correction $E_{\text{LHY}}$ are of great interest due to their deep connections with many-body correlation and quantum fluctuations. With the help of magnetic Feshbach resonances to control the scattering length, the influences of the LHY correction have been studied in various ultracold systems [2–6]. However, typically LHY effects are clearly visible only in the strongly interacting regime with large scattering lengths when $E_{\text{LHY}}$ becomes more or less comparable to MF energy $E_{\text{MF}}$.

The situation can be very different in a double BEC with repulsive intraspecies interactions and a tunable attractive interspecies interaction. In such a system, the total $E_{\text{MF}}$ of the system can be largely canceled or even become negative while the positive $E_{\text{LHY}}$ is nearly intact. As $E_{\text{LHY}}$ is now dominant, its effects become pronounced even though the system is still in the weakly interacting regime [7, 8]. At $E_{\text{MF}}$ near zero, the double BEC forms the so-called LHY fluid, which has been studied recently [8, 9]. For negative $E_{\text{MF}}$, the system can enter the quantum liquid droplet phase with a signature self-bound behavior in free space [10–13]. Quantum droplets have also been observed in some single-species ultracold lanthanoid systems in which $E_{\text{MF}}$ can be balanced by the dipolar interaction [14–20].

In this work, we study in two different ways the LHY effects in a double BEC of $^{23}$Na and $^{87}$Rb atoms with tunable attractive interspecies interactions. First, we observe the heteronuclear quantum liquid droplet in free space with more than $10^4$ atoms when the interspecies Na-Rb scattering length is tuned into the mean-field collapse regime. Under optimized conditions, a low-number-density droplet with lifetime exceeding the observation time is observed. We also investigate the liquid-to-gas phase transition and obtain the critical atom numbers at the phase boundary. Second, we measure the release energies of two types of gas-phase mixtures, the pure in-trap gases. However, its effects are often elusive due to the typically much larger influence of the MF energy. In this work, we study an ultracold mixture of $^{23}$Na and $^{87}$Rb with negative $\delta g$ to characterize the total $E_{\text{LHY}}$, with $\overline{g} = (g_{11} + g_{22})/2$. For the current system, the critical magnetic field for $\delta g = 0$ (and also $\delta g = 0$) is $B_c = 350.027$ G, which corresponds to a critical interspecies scattering length $a_{12} = 60.2a_0$. As shown in Fig. 1(a) (lower panel), for each value of $\delta g < 0$, the double BEC will undergo a transition from gas phase to liquid-to-gas phase transition shows an anomalous expansion featuring a larger release energy for increasing mean-field attractions.
droplet phase as the atom numbers are increased. With our atom numbers around $10^4$ for both species, the theory predicts an observation window for the droplet phase for $\delta g$ from $-0.110$ to $-0.247$ (349.910 G to 349.780 G). For $\delta g$ from 0 to $-0.110$, droplet formation is still possible but atom numbers much larger than currently available are needed.

In the first experiment, we study the Na-Rb quantum droplet in free space by releasing the sample from the optical trap. We probe the system during the time of flight (TOF), as depicted in the inset of Fig. 1(a). To probe the atoms in situ at each TOF, we implement a two-species high-field detection protocol which consists of a partial optical pumping process followed by standard absorption imaging on the cycling transitions [26]. This partial imaging method is necessary as the droplets have very high optical depth and are difficult to detect directly [11, 27]. Both the partial optical pumping and the absorption imaging are calibrated using standard methods [28, 29]. The measured resolutions (1/$\sqrt{\tau}$ half Gaussian widths) of our imaging system are 0.6 $\mu$m and 0.8 $\mu$m for $^{23}$Na at 589 nm and $^{87}$Rb at 780 nm, respectively, which are just enough to resolve the droplet. To maintain the imaging resolutions, we mount the objective and the probe light optics on high-precision vertical translational stages to keep the optical axis of the imaging system always aligned with the droplet.

While shutting down the optical trap provides a direct way of probing the droplet in free space, the non-adiabatic nature of the process can cause problems. Due to the confinement, the in-trap sample is smaller in size than the free-space droplet in its ground state, while the total energy of the system is much larger. In the worst scenario, the energy of the initial state upon release from the trap is larger than the free-space droplet in its ground state, while the total energy of the system is much larger. In the worst scenario, the energy of the initial state upon release from the trap is larger than the energy barrier of the expansion and a stable droplet can never be formed [30]. To mitigate this problem, the crossed optical dipole trap is configured in a nearly spherical shape with measured trap oscillation frequencies of 78 Hz (86 Hz) for $^{87}$Rb ($^{23}$Na). This is in accordance with the understanding that a quantum droplet with isotropic short-range interactions should be spherical in free space. In addition, a carefully designed magnetic field control sequence is used to improve the mode matching [30]. These steps allow us to observe droplet formation reliably for $\delta g$ from $-0.146$ to $-0.247$. However, for $\delta g$ from $-0.110$ to $-0.146$, due to the smaller binding energy, droplets can be observed only by a more sophisticated mode-matching method, aided by fast magnetic field quenching at the instant of releasing the samples from the trap [30]. For this method to work, the starting magnetic field must be selected carefully so that the size of the in-trap sample matches that of the free-space droplet at the end of the magnetic field quenching.

Figure 1(b) shows a side-by-side comparison of the $^{23}$Na and $^{87}$Rb clouds in the gas phase and the droplet phase following the TOF. The signature self-bound behavior of the droplet can be observed clearly by compar-
ing its dramatically different TOF expansion with that in the gas phase. For $\delta g = -0.173$ (349.849 G), where the droplet phase is expected, the sizes of both clouds stay nearly the same during the TOF. For $\delta g = +0.322$ (350.451 G), by contrast, the system remains in the gas phase, and the sizes increase steadily with TOF.

To extract quantitative information, we fit the images with 2D Gaussian functions. In the droplet, the size should be the same for the two species; their densities and thus numbers should follow the ratio $N_2/N_1 = \sqrt{g_{11}/g_{22}} = 1.43$ [7]. When this ratio is not maintained, the droplet part shows up as a dense central peak, and the excess atoms of one species appear as a much larger-sized and expanding gaseous background surrounding the droplet [inset of Fig. 1(c)]. For this kind of “bimodal” distribution, the droplet parameters are extracted with a double 2D Gaussian fitting. Fig. 1(c) shows the starkly different expansion behaviors in the droplet and the gas phases obtained from the images in Fig. 1(b).

For the droplets formed by direct trap release from $\delta g = -0.146$ to $-0.247$, we observe two distinctively different dynamics in the evolution of the $^{23}$Na and $^{87}$Rb samples during the TOF. As an example, Fig. 2(a), (b) and (c) show the sizes, atom numbers, and number ratio of the droplet sample for $\delta g = -0.169$ (349.852 G). During the first 10 ms, the $^{23}$Na and $^{87}$Rb sizes increase very little, while atom losses are observed for both species. Bimodal distributions are observed from 0 ms to 5 ms as the initial number ratio is far from 1.43. After 5 ms expansion, the gaseous atoms surrounding the droplet are already too dilute to be detected.

After about 10 ms, the sample sizes start to increase while the atom numbers stay nearly constant. This is consistent with a phase transition from droplet to gas when the atom numbers are reduced to below the critical values [see Fig. 1(a)]. We fit the size evolution empirically with $\sigma(t > t_0) = \sqrt{\sigma_0^2 + v^2(t - t_0)^2}$ and $\sigma(t < t_0) = \sigma_0$, and obtain a lifetime in the droplet phase of about $t_0 = 7$ ms. Here $v$ is the expansion velocity of the gas-phase sample. Similarly, as illustrated in Fig. 2(b), the critical atom numbers for the phase transition can be obtained by fitting the $^{23}$Na and $^{87}$Rb number evolution data with an exponential decay function with the critical number as the offset.

For several values of $\delta g$ between $-0.110$ and $-0.146$, we have created longer-lived droplets by the magnetic field quenching method. As shown in Fig. 2(d), (e) and (f), during the accessible TOF, the droplet size stays nearly the same although number losses are still observed. After 10 ms, the number ratio becomes close to 1.43 and the number loss slows down significantly. As the lifetime is longer than the usable TOF of 18 ms, we have not been able to measure the real lifetime and the critical numbers in this range of $\delta g$. More detailed investigations, e.g., by levitating the droplet, are warranted in the near future.

Figure 3 shows the critical $^{23}$Na and $^{87}$Rb atom numbers for $\delta g$ from $-0.146$ to $-0.247$. Although the range of $\delta g$ is small, a four-fold change in the measured critical numbers is observed. The critical numbers calculated using coupled eGPEs with the LHY term included (dashed curves) show large discrepancies with the measurements. The agreement is greatly improved by also including the small post-compensation residual magnetic field gradient in the eGPEs (solid curves); the additional term nearly doubles the critical numbers. This can be understood from the different magnetic dipole moments and masses of $^{23}$Na and $^{87}$Rb, which cause their centers of mass to separate in a magnetic field gradient [30]. This decreases the density overlap and lowers the attractive interspecies mean-field energy while leaving the intraspecies energy nearly intact. Effectively, this increases the critical numbers compared to the ideal case of zero gradient.

A major cause of the atom losses is three-body recombination as a result of the high number densities in the droplet [10–12, 30]. For droplets with $\delta g$ from $-0.146$ to $-0.247$, another possible loss mechanism is self-evaporation due to the imperfect matching between in-trap and free-space modes [31]. The short lifetimes in this region are the combined result of these loss mechanisms. In contrast, the droplet at $\delta g = -0.141$ [see Fig. 2(d), (e), and (f)] has relatively lower number densities and is formed with nearly optimal mode matching, and is thus longer lived. Nevertheless, for both cases, the stabilized number ratios after 10 ms TOF are very close to 1.43 despite the different creation procedures and the

![FIG. 2. Evolution of the Na-Rb droplet in free space. (a), (b), and (c) show the size, atom numbers, and the $^{87}$Rb to $^{23}$Na number ratio at $\delta g = -0.169$ (349.852 G) following the TOF. The droplet is created by directly releasing the sample from the trap. The vertical bar marks the approximate time of the liquid-to-gas phase transition. (d), (e), and (f) show the evolution for the droplet created with the additional magnetic field quenching for $\delta g = -0.141$ (349.880 G). The red dashed lines in (c) and (f) mark the theoretical number ratio $N_2/N_1 = 1.43$.](image-url)
We now turn to the gas-phase double BEC and release the sample directly from the trap (without the additional magnetic field quenching) for $\delta g$ from +0.322 to -0.146. To characterize the LHY effect, we measure the release energy $E_{\text{rel}} = E_{\text{kin}} + E_{\text{int}}$ from the TOF expansion [30, 32, 33]. Here $E_{\text{kin}}$ is the quantum pressure and $E_{\text{int}} = E_{\text{MF}} + E_{\text{LHY}}$ is the total interaction energy. When $E_{\text{MF}}$ is tuned to zero, $E_{\text{LHY}}$ becomes the only interaction term in $E_{\text{rel}}$. For negative $E_{\text{MF}}$, the fact that the sample expands rather than collapses is also a direct manifestation of the LHY effect.

We prepare the trapped double BEC and measure $E_{\text{rel}}$ from the TOF expansion velocities of the two species [30, 32] for several different values of $\delta g$. The resulting $E_{\text{rel}}$ is shown as open squares in Fig. 4. In general, $E_{\text{rel}}$ depends on $\delta g$, $N_1$ and $N_2$, and the density overlap between the two species. However, in this range of $\delta g$, the densities of the double BEC are still rather high even in the gas phase, and significant three-body losses are observed during the TOF. Thus, it is difficult to maintain constant $N_1$ and $N_2$ during the TOF for different $\delta g$, even though great efforts are made to keep the initial atom numbers in the trap fixed. Nevertheless, since $E_{\text{rel}}$ is a measure of the energy per atom, it is not affected severely by the loss.

We calculate $E_{\text{rel}}$ with the eGPEs for the corresponding atom numbers at the end of the TOF and find good agreement for $\delta g \gtrsim 0$, corresponding to $E_{\text{MF}} \gg E_{\text{LHY}}$ or $E_{\text{MF}} \approx 0$ (red solid curve in Fig. 4). We note that, without the LHY term, the calculation fails for $\delta g < 0$ due to collapse of the double BEC (blue solid curve in Fig. 4). At $\delta g \approx 0$, where $E_{\text{MF}}$ almost cancels, the energy difference between the two calculations is about 1 nK. This is essentially the magnitude of $E_{\text{LHY}}$, if we assume $E_{\text{kin}}$ does not change dramatically between the two cases.

The gas-phase mixture formed following the liquid-to-gas phase transition is also of great interest. As shown in Fig. 2(a), its expansion velocity can be measured and converted into another $E_{\text{rel}}$ even though there is no trap involved. Following the number losses, the total energy of the system changes from negative in the droplet phase to positive in the metastable and eventually gas phase. $E_{\text{rel}}$ here is thus just the sum of $E_{\text{kin}}$, $E_{\text{MF}}$, and $E_{\text{LHY}}$ at the phase transition point [30]. The measured $E_{\text{rel}}$ is shown in Fig. 4 as solid circles for $\delta g$ from -0.146 to -0.247. It has the opposite dependence on $\delta g$ from that observed for the gas-phase mixture released from the trap. This is similar to previous observations on the expansion dynamics of the erbium dipolar system [17].

This behavior can be qualitatively understood from the competition between $E_{\text{LHY}}$, $E_{\text{kin}}$, and $E_{\text{MF}}$ for the droplet near the phase transition point. As $\delta g$ becomes more negative, the critical atom numbers at the phase transition point become smaller, and the sample also shrinks. The positive $E_{\text{LHY}}$ and $E_{\text{kin}}$ terms increase faster than the negative $E_{\text{MF}}$ term decreases. The measured $E_{\text{rel}}$ thus increases for more negative $\delta g$. We note that, without $E_{\text{LHY}}$, the magnitude of $E_{\text{MF}}$ is larger than $E_{\text{kin}}$ and the system collapses. This picture is confirmed semi-quantitatively by the eGPE calculation, shown by
the red dashed curve in Fig. 4. As a comparison, a variational calculation (magenta short-dashed curve) using the experimentally measured atom numbers and the Gaussian ansatz, is also shown; this actually agrees better with the experimental data. The deviation between the experiment and the eGPE calculation may be due to the inaccuracy in determining the transition point.

In conclusion, we have studied the heteronuclear BEC mixture of $^{87}$Rb and $^{23}$Na atoms with attractive inter-perspeces interactions, under conditions where the role of the LHY correction is amplified. The signatures of the LHY correction manifest clearly in both the self-bound behavior of the free-space quantum liquid droplet and the expansion of the gas-phase mixtures. Although the observation time is limited by the detection method, our result shows that heteronuclear droplets can be long-lived. This will allow quantitative studies on the fundamental properties of the quantum droplet, such as the existence of a possible Bose pairing mechanism [34, 35] with mass-imbalanced constituents. Another interesting topic is quantum droplets in lower dimensions and at the crossover between different dimensionalities [36–38]. The $^{23}$Na and $^{87}$Rb system here also holds great promise in creating large quantum liquid droplets with more than $10^6$ atoms [39, 40]. In this so far unachieved regime, the droplet features a large core with constant density, and various peculiar collective excitation may be investigated [7].

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See supplementary materials at [url to be added] which includes references [7].

SUPPLEMENTAL MATERIAL

Magnetic Field Gradient Compensation

An important technical issue for observing the free-space droplet is the spatial varying magnetic field experienced by the droplet during the TOF. Due to the different magnetic dipole moments of $^{23}\text{Na}$ ($\mu_{1}$ = 1.084 MHz/G) and $^{87}\text{Rb}$ ($\mu_{2}$ = 0.837 MHz/G) near $B_{0}$, a moderate gradient and curvature may generate a differential force large enough to tear the droplet apart. With the pair of Feshbach coils only, the measured magnetic field curvature near 347 G is 1.4 G/cm$^2$, and the averaged magnetic field gradient is about 0.6 G/cm. Experimentally, we observe the $^{23}\text{Na}$ and $^{87}\text{Rb}$ atomic clouds separating from each other following the TOF. To mitigate this problem, we placed another coil, with its current dynamically controlled following the TOF, on top of the Feshbach coil. This simple improvement reduces the magnetic field gradient to 0.11 G/cm and the averaged magnetic field gradient variation during the 18 ms TOF from ±10 mG to ±3 mG which corresponds to a $a_{12}$ change of less than 0.26 $a_{0}$.

In the eGPEs, the magnetic field gradient is included as opposite direction linear potentials to the two species in the center-of-mass coordinate. According to the simulation, this small magnetic field gradient actually doubles the critical atom numbers.

In-trap and free-space mode matching

During the release of the double BEC sample from the optical trap, the trap energy suddenly is removed sud-
FIG. S1. Droplet formation by directly releasing the trapped sample. The blue dashed curves represent $E_{\text{tot}} = E_{\text{kin}} + E_{\text{pot}} + E_{\text{int}}$ of the trapped double BEC, and the red solid curves are $E_{\text{tot}}$ in free space (i.e., $E_{\text{kin}} + E_{\text{int}}$). (a) For very small $|\delta g|$, the free-space $E_{\text{tot}}$ (the red open circle) is higher than the barrier height on the large size side (the red solid dot). In this case, the sample will keep expanding and never forms the droplet. (b) For $|\delta g|$ large enough, the sample does not have enough energy and will be confined near the energy minimum to form the droplet.

As depicted in Fig. S1(b), although droplet can be observed after these improvements for $|\delta g|$ large enough, the mode matching is not perfect. For $|\delta g|$ large enough, the magnetic field is ramped to a target value within 5 ms and the magnetic field holds here for only 10 ms. Afterwards, the magnetic field is ramped to a target value within 5 ms before the droplet is detected in free space.
\( \delta q = -0.110 \), the liquid-to-gas phase transition is observed after about 7 ms. This short lifetime is probably limited by the atom numbers since at this \( \delta g \), the critical atom numbers are much larger.

### Three-body loss

As discussed in the main text, the major losses of atom number are from three-body loss as a result of the high density of the droplet sample. We observe a faster loss of \(^{87}\text{Rb} \) than that of \(^{23}\text{Na} \) at almost all magnetic fields. We believe this is due to the larger three body loss rate constant \((7.2 \times 10^{-30} \text{ cm}^6/\text{s})\) of the \(^{87}\text{Rb} \) BEC than that of the \(^{23}\text{Na} \) BEC \((1.1 \times 10^{-30} \text{ cm}^6/\text{s})\) [41, 42].

While the three-body loss rate constants for condensed \(^{87}\text{Rb} \) and \(^{23}\text{Na} \) atoms are well known [41, 42], that between \(^{23}\text{Na} \) and \(^{87}\text{Rb} \) with the weak interspecies interaction near \( B_c \) is unknown. But from our previous few-body investigations [43], no heteronuclear Efimov resonances are expected near this region; thus, we can assume that the heteronuclear three-body loss should have a similar rate as single species \(^{87}\text{Rb} \) or \(^{23}\text{Na} \) samples.

### Release energies

![Graph](image)

**FIG. S3.** The release energies. (a) Origin of \( E_{rel} \) for the gas released from the trap. The blue dashed curve is the in-trap total energy \( E_{tot} = E_{pot} + E_{kin} + E_{int} \), and the red solid curve is \( E_{tot} \) without \( E_{pot} \) when the sample is suddenly released from the trap. (b) \( E_{rel} \) for the case following the liquid-to-gas phase transition. The blue and orange dashed curves are \( E_{tot} \) of the stable and meta-stable droplets, respectively. The red solid curve is \( E_{tot} \) just on the phase transition point, where the local minimum disappears. For both cases, following the size increase, the quantum pressure \( E_{kin} \) and the interaction energy \( E_{int} \) are converted to the kinetic energy of the atoms.

For the double BEC system studied here, the average release energy is defined as \( E_{rel} = \left( \frac{1}{2} m_1 v_1^2 N_1 + \frac{1}{2} m_2 v_2^2 N_2 \right)/\left( N_1 + N_2 \right) \), where \( v_i \) is the expansion velocity. Fig. S3 illustrates schematically the different origins of \( E_{rel} \) for the in-trap gas and the gas formed from the droplet. For the first case [Fig. S3(a)], \( E_{rel} \) is dominated by \( E_{MF} \) and decreases for smaller \( \delta g \). For the gas from phase transition case [Fig. S3(b)], the total energy of the sample and thus \( E_{rel} \) increases when \( \delta g \) gets more negative.

Experimentally, the RMS sizes are obtained from fitting to the absorption images. Different fitting functions are used for the two cases. For the sample directly released from the trap, the images are fitted with the parabola function in accordance with the Thomas-Fermi approximation for BECs with more than \( 10^4 \) atoms. For the gas mixtures formed following the liquid-to-gas transition, the Gaussian function, which is closer to the small atom number sample profiles, is used.

### Numerical Simulation

For the condensate mixture of \(^{23}\text{Na} \) and \(^{87}\text{Rb} \) (denoted as species 1 and 2 hereafter, respectively) considered here, the coupled extended Gross-Pitaevskii equations (eGPEs) including the LHY correction reads

\[
i \hbar \frac{\partial \psi_i}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_i} + V_i + \mu_i (n_1, n_2) \right) \psi_i \tag{S1}\]

with \( m_i \) the atomic mass, \( n_i \) the number density, and

\[
\mu_i = g_{ii} n_i + g_{ij} n_j + \frac{\delta \mathcal{E}_{\text{LHY}}}{\delta n_i}, \ (i \neq j). \tag{S2}
\]

As introduced in [7, 44], the LHY term for mass imbalanced system can be described as

\[
\mathcal{E}_{\text{LHY}} = \frac{8}{15 \pi^2} \left( \frac{m_1^{3/2} (g_{11} n_1)^{5/2}}{g_{22} n_2/g_{11} n_1} \right)^{3/5} f(\gamma, x, y) \tag{S3}
\]

with \( \gamma = m_2/m_1 \), \( x = g_{21}^{3/2}/g_{22} g_{11} \) and \( y = g_{22} n_2/g_{11} n_1 \). The dimensionless parameter \( f(\gamma, x, y) \) represents the renormalized integral with only numerical solution for the mass imbalanced case.

For the in-trap case, the \( V_i \) term in Eq. S1 includes both the trapping potential and the contribution from the residual magnetic field gradient. In free space, it is only from the residual magnetic field gradient. The gradient \( \partial B/\partial y \) is mainly along the vertical (y) direction. In the center-of-mass coordinate, the differential magnetic dipole moments lead to opposite direction linear potentials to the two species,

\[
V_i = \left( -\mu_i \frac{\partial B}{\partial y} - a_c m_i \right) y \tag{S4}
\]

where \( a_c \) is the acceleration of center-of-mass

\[
a_c = \frac{\left( \mu_{b1} N_1 + \mu_{b1} N_2 \right)}{N_1 m_1 + N_2 m_2} \frac{\partial B}{\partial y} \tag{S5}
\]