An impurity in a heteronuclear two-component Bose-Bose mixture

Main reference: G. Bighin, A. Burchianti, F. Minardi, and T. Macrì, arXiv:2109.07451

Giacomo Bighin

October 21th, 2021

Introduction: impurities and Bose-Bose mixtures

The problem of an **impurity particle moving through a bosonic medium** is a fundamental paradigm in many-body physics, from the early years when the polaron quasiparticle was introduced to describe an electron in a crystal environment, to recent breakthrough experiments with ultracold atoms.

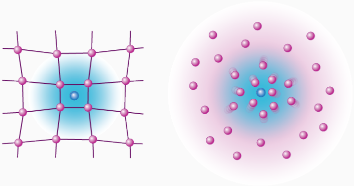

Image: APS/Carin Cain.

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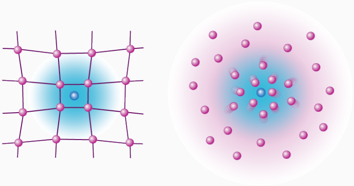

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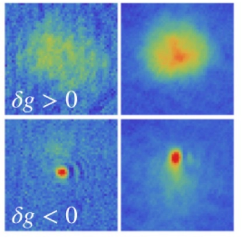

C. D'Errico *et al.*, Phys. Rev. Research **1**, 033155 (2019).

A **Bose-Bose mixture** consists of a mixture of two different bosonic atomic species. Quite involved phase diagram, including the remarkable **quantum droplet** state, i.e. a liquid-like self-bound state. Quantum droplets have been observed in a homonuclear spin mixture of ^{39}K, both in the presence of an external potential and in free space, as well as in a **heteronuclear mixture of ^{41}K and ^{87}Rb**.

The system: Hamiltonian

Interacting Bose-Bose mixture:

$$\hat{H}_{\mathsf{bb}} = \int \mathrm{d}^3 r \sum_{i=1,2} \hat{\phi}_i^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m_i} + \frac{g_{ii}}{2}|\hat{\phi}_i(\mathbf{r})|^2\right)\hat{\phi}_i(\mathbf{r}) + g_{12}\int \mathrm{d}^3 r |\hat{\phi}_1(\mathbf{r})|^2|\hat{\phi}_2(\mathbf{r})|^2$$

where $\hat{\phi}_i$, $\hat{\phi}_i^\dagger$ $(i = 1, 2)$ are bosonic field operators acting on two different bosonic species, m_i are the masses of each species and g_{ij} is the contact interaction strength between species i and species j.

Impurity in the mixture:

$$\hat{H}_{\mathsf{I}} = \frac{\hat{\mathbf{P}}^2}{2m_{\mathsf{I}}} + \sum_i g_{Ii} \int \mathrm{d}^3 r\, \rho(\mathbf{r})\, |\hat{\phi}_i(\mathbf{r})|^2$$

where g_{Ii} is the interaction between the impurity and the species i and $\rho(\mathbf{r}) = \delta^{(3)}(\mathbf{r} - \hat{\mathbf{R}})$.

Many parameters! Five different interaction strengths: g_{11}, g_{22}, g_{12}, g_{I1}, g_{I2}.

Bose-Bose mixture: miscible and immiscible phases, collapse

Mean-field description: one can obtain conditions for the stability of the ultracold mixture from a Gross-Pitaevskii approach[1], considering $g_{11}, g_{22} > 0$ and varying the sign of g_{12}:

- When $g_{12} > \sqrt{g_{11} g_{22}}$ phase separation occurs.
- When $-\sqrt{g_{11} g_{22}} < g_{12} < \sqrt{g_{11} g_{22}}$ the system is in a miscible state.
- When $-\sqrt{g_{11} g_{22}} > g_{12}$ the system undergoes collapse.

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Is this the full story? Can beyond-mean-field effect alter this picture?

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A Bose-Bose mixture in the collapsing regime can be stabilized by quantum fluctuations. The interplay between mean-field attraction and beyond-mean-field repulsion remarkably leads to a stable **droplet** state.

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Quantum Mechanical Stabilization of a Collapsing Bose-Bose Mixture

D. S. Petrov
Université Paris-Sud, CNRS, LPTMS, UMR8626, Orsay, F-91405, France
(Received 28 June 2015; published 7 October 2015)

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What makes a liquid a liquid?

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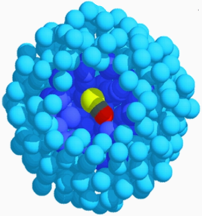

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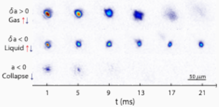

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Self-bound quantum droplets: from quantum gases to quantum liquids

What makes a liquid a liquid?

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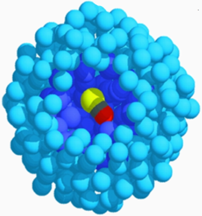

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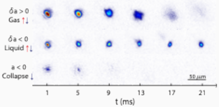

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In most well known cases, it is a balance between repulsive and attractive interatomic forces!

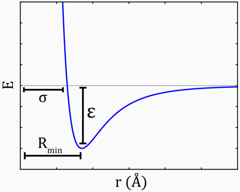


Image credit: Wikibooks, *"Molecular simulation"*.

Self-bound quantum droplets in a Bose-Bose mixture

Single-component Bose gas:

$$\frac{E}{V} = \frac{gn^2}{2}\left(1 + \frac{128\sqrt{na^3}}{15\sqrt{\pi}} + \dots\right)$$

with the LHY correction due to the zero-point motion of Bogoliubov excitation, i.e. a purely quantomechanical effect.

Two-component Bose mixture:

$$\frac{E}{V} = \sum_{ij} \frac{g_{ij} n_i n_j}{2} + \frac{8}{15\pi^2} m_1^{3/2} (g_{11} n_1)^{5/2} f\left(\frac{m_2}{m_1}, \frac{g_{12}^2}{g_{11} g_{22}}, \frac{g_{22} n_2}{g_{11} n_1}\right)$$

and there can be competition between the mean-field attraction $\propto n^2$ and beyond mean-field repulsion $\propto n^{5/2}$, also in the weakly-interacting regime.

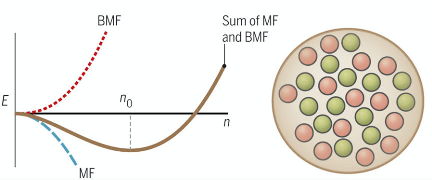
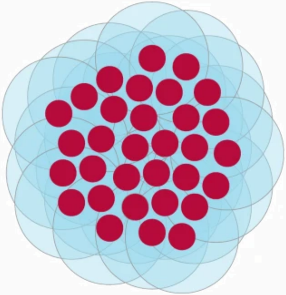


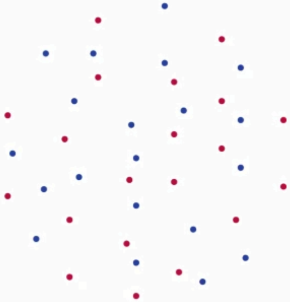
Image credit: Science.

Self-bound quantum droplets in a Bose-Bose mixture

“Classical” van der Waals paradigm for a droplet



Quantum droplet

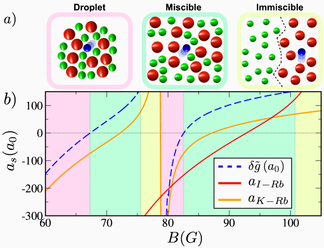


What about **dipolar droplets** (Stuttgart, Innsbruck)? There are great differences, but the basic mechanism – mean-field attraction compensated by beyond-mean-field effects – is essentially the same.

Images from D.S. Petrov, Nat. Phys. **14**, 211 (2018).

A closer look at the Bose-Bose mixture

We consider a **heteronuclear ^{41}K-^{87}Rb Bose mixture**, on top of which which consider a dilute third component realized with a different hyperfine state of ^{41}K – which we shall dub the ‘I’ species. In the impurity limit for the third component, the system is described by five scattering lengths, namely $a_{\text{K-K}}$, $a_{\text{K-Rb}}$, $a_{\text{Rb-Rb}}$, $a_{\text{I-K}}$, $a_{\text{I-Rb}}$. The behaviour of $a_{\text{I-Rb}}$, and $a_{\text{K-Rb}}$ as a function of the magnetic field B in the range between 60 and 105 G.



Scattering length calculations: A. Simoni.

The other three scattering lengths are almost constant in the range considered, i.e. $a_{\text{K-K}} \simeq a_{\text{I-K}} \simeq 62a_0$, $a_{\text{Rb-Rb}} \simeq 100.4a_0$.

The liquid-gas transition parameter $\delta g = g_{\text{K-Rb}} + \sqrt{g_{K-K} g_{\text{Rb-Rb}}}$, allows us to chart the Bose mixture phase diagram: as the magnetic field is varied in the aforementioned range, the mixture goes through the droplet, miscible and immiscible phases.

Theoretical framework: Bogoliubov approach to a Bose-Bose mixture

Generalization of the usual Bogoliubov transformation: at first we expand the bosonic field in plane waves as

$$\hat{\phi}_1(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \alpha_{\mathbf{q}} \qquad \hat{\phi}_2(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \beta_{\mathbf{q}}$$

and then we expand in the fluctuations around the ground state of the condensate

$$\alpha_{\mathbf{q}} = (2\pi)^3 \sqrt{n_1} \delta(\mathbf{q}) + A_{\mathbf{q}\neq 0}, \qquad \beta_{\mathbf{q}} = (2\pi)^3 \sqrt{n_2} \delta(\mathbf{q}) + B_{\mathbf{q}\neq 0} \ .$$

Finally, a rotation brings the Hamiltonian in diagonal form, at the expense of introducing the 'new' field operators $\hat{a}_{\mathbf{k}}$, $\hat{b}_{\mathbf{k}}$, whose excitations are given by the Bogoliubov-like dispersions: $\omega_{\mathbf{k}}^{(A)}$, $\omega_{\mathbf{k}}^{(B)}$.

$$\begin{pmatrix} \hat{A}_{\mathbf{k}} \\ \hat{A}^\dagger_{-\mathbf{k}} \\ \hat{B}_{\mathbf{k}} \\ \hat{B}^\dagger_{-\mathbf{k}} \end{pmatrix} = \mathbb{M}_{ij} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{a}^\dagger_{-\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \\ \hat{b}^\dagger_{-\mathbf{k}} \end{pmatrix}$$

Result: the Hamiltonian is diagonal in the new field operators, however the impurity coupling to one component will correspond to coupling to a combination of $\hat{a}_{\mathbf{k}}$, $\hat{a}^\dagger_{\mathbf{k}}$, $\hat{b}_{\mathbf{k}}$ and $\hat{b}^\dagger_{\mathbf{k}}$.

Miscible phase: Hamiltonian

Impurity and bosons: $\hat{H}_{\text{imp}} = \frac{\hat{\mathbf{P}}^2}{2m_I}$ $\qquad H_{\text{bos}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}}^{(A)} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \omega_{\mathbf{k}}^{(B)} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}$

Fröhlich-level interaction: $\hat{H}^{(1)}_{\text{imp-bos}} = \sum_{\mathbf{k}\neq 0} e^{\mathrm{i}\mathbf{k}\cdot\hat{\mathbf{R}}} [U_A(\mathbf{k})(\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{-\mathbf{k}}) + U_B(\mathbf{k})(\hat{b}_{\mathbf{k}} + \hat{b}^\dagger_{-\mathbf{k}})]$

It has been shown[2] that terms bilinear in the bosonic operators, describing the scattering of the impurity off the condensate, can be very important for an accurate description of the physics of quantum impurities in ultracold gases. For this reason, we extend our description including bilinear terms

$$H^{(2)}_{\text{imp-bos}} = \sum_{\substack{\mathbf{k},\mathbf{k}' \\ i=A,B}} e^{\mathrm{i}(\mathbf{k}+\mathbf{k}')\cdot\hat{\mathbf{R}}}\, \Psi_a(\mathbf{k}')\mathbb{Q}^i_{ab}(\mathbf{k}',\mathbf{k})\Psi_b(\mathbf{k})$$

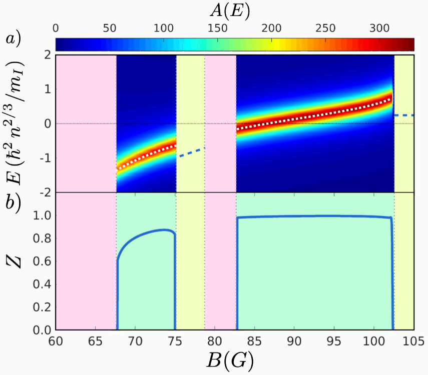
having grouped the creation and annihilation operators into a spinor-like object $\Psi(\mathbf{k}) = (a_{\mathbf{k}}\ a^\dagger_{-\mathbf{k}}\ b_{\mathbf{k}}\ b^\dagger_{-\mathbf{k}})^T$.

[2] Y.E. Shchadilova *et al.*, Phys. Rev. Lett. **117**, 34 (2016). Y. Ashida *et al.*, Phys. Rev. B **97**, 060302(R) (2018).

Miscible phase: variational Ansatz and spectral function

The full Hamiltonian $\hat{H} = H_{\text{bos}} + H_{\text{imp}} + \hat{H}^{(1)}_{\text{imp-bos}} + H^{(2)}_{\text{imp-bos}}$ is then solved using a well-established approach: a Lee-Low-Pines transformation bring a to a frame of reference co-moving with the impurity, whose wavefunction is then modeled by a coherent-state variational Ansatz:

$$|\Psi(t)\rangle = e^{i\phi(t)}\, e^{\sum_{\mathbf{k}} \alpha_{\mathbf{k}}(t) a^{\dagger}_{\mathbf{k}} - h.c.}\, e^{\sum_{\mathbf{k}} \beta_{\mathbf{k}}(t) b^{\dagger}_{\mathbf{k}} - h.c.}\, |0\rangle^{A} \, |0\rangle^{B}$$



Spectral function of the impurity as a function of the (rescaled) energy E and of the magnetic field B. The coupling of the polaron to the K component is always repulsive, whereas the coupling to the Rb component changes from attractive to repulsive at around $92.8\ G$.

Droplet phase: Gross-Pitaevskii approach

To study the effect of an impurity in the droplet phase we assume that, within the Gross-Pitaevskii framework, the two components are described by a complex field $\psi_i(\mathbf{r})$ with the associated energy functional

$$E_{bb}[\phi_i] = \int \mathrm{d}^3 r \sum_{i=1,2} \left(\frac{\hbar^2 |\nabla \phi_i|^2}{2m_i} + \frac{g_{ii}}{2} |\phi_i|^4 \right) + g_{12} |\phi_1|^2 |\phi_2|^2 + \\ + \frac{8}{15\pi^2 \hbar^3} \left(m_1^{\frac{3}{5}} g_{11} |\phi_1|^2 + m_2^{\frac{3}{5}} g_{22} |\phi_2|^2 \right)^{\frac{5}{2}}$$

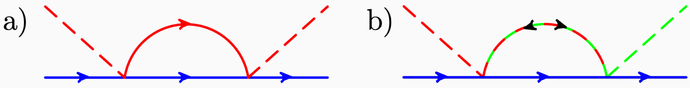
where the last term is the beyond mean-field interaction for a general two-component mixture. The impurity interaction with the Bose mixture is described by the energy functional

$$E_I[\phi_i, \psi] = \int \mathrm{d}^3 r \frac{\hbar^2 |\nabla \psi|^2}{2m_I} + \left(g_{ID} |\phi(\mathbf{r})|^2 + \mathscr{E}_{\mathsf{BMF}}(\mathbf{r}) \right) |\psi(\mathbf{r})|^2$$

The last term $\mathscr{E}_{\mathsf{BMF}}(\mathbf{r})$ is the beyond mean-field interaction for a general two-component mixture.

Droplet phase: beyond-mean-field impurity-mixture interaction

We obtain $\mathscr{E}_{\mathsf{BMF}}(\mathbf{r})$ by means of perturbation theory in the small parameters (a_{Ii}/ξ_i), $i = 1, 2$, where $\xi_i = 1/\sqrt{8\pi n_i a_{ii}}$ is the healing length for the i-th component, following a perturbative approach[3]. Novelty: diagrams mixing different normal components in the condensate.



The energy correction at the second order reads

$$\mathscr{E}_{\mathsf{BMF}} = \frac{1}{1+\alpha}\left(\frac{2\pi\hbar^2\xi_1\, n}{\mu_{I1}}\right)\left(\frac{a_{I1}}{\xi_1}\right)^2\frac{m_1}{\mu_{I1}}I_1 + \frac{\alpha}{1+\alpha}\left(\frac{2\pi\hbar^2\xi_2\, n}{\mu_{I2}}\right)\left(\frac{a_{I2}}{\xi_2}\right)^2\frac{m_2}{\mu_{I2}}I_2,$$

for some dimensionless integrals I_1 and I_2.

[3] One component case: R.S. Christensen *et al.*, Phys. Rev. Lett. **115**, 160401 (2015).

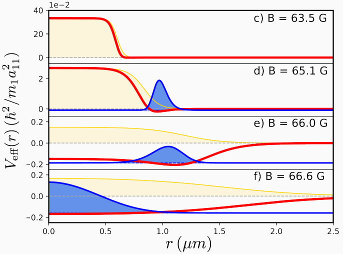
Droplet phase: Gross-Pitaevskii equations

We finally obtain the (rescaled) Gross-Pitaevskii equations to be solved numerically for the impurity-droplet system (the impurity has mass m_1)

$$\begin{cases} \mathrm{i}\frac{\partial\psi}{\partial t} & = & \left(-\frac{\nabla^2}{2} + g_{ID}|\phi|^2 + \mathscr{E}_{\mathsf{BMF}}\right)\psi(\mathbf{r},t) \\ \\ \mathrm{i}\frac{\partial\phi}{\partial t} & = & \left(-\frac{\nabla^2}{2m^*} + g_{ID}|\psi|^2 + g_{MF}|\phi|^2 + g_{LHY}|\phi|^3\right)\phi(\mathbf{r},t). \end{cases}$$

where we introduced the effective couplings g_{ID}, g_{MF}, g_{LHY} and an effective mass m^*.

Droplet phase: results

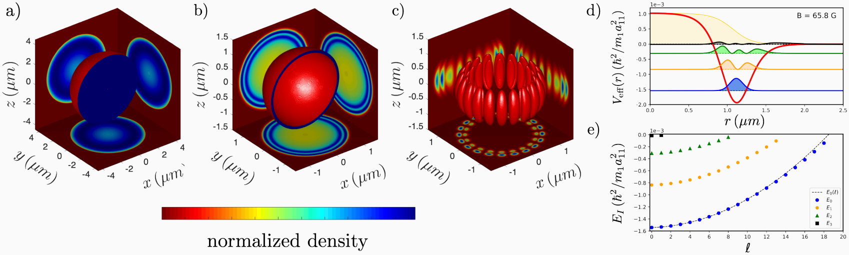


Quite a rich phenomenology arises, as for $B = 63.5\ G$ the potential, even though it has a small attractive region, does not support bound states in three dimensions not allowing for an impurity to be bound to the droplet. Also note the effective potential exerted by the mixture on the impurity, $V_{\text{eff}}(\mathbf{r}) = g_{ID}|\phi(\mathbf{r})|^2 + \mathscr{E}_{\text{BMF}}(\mathbf{r})$.

As the magnetic field is increased, for $B = 65.1\ G$ and for $B = 66.0\ G$ we observe that the impurity is localized at the surface of the droplet at a distance $r \approx 1\mu m$ form the center; we stress that the beyond-mean-field correction $\mathscr{E}_{\text{BMF}}$ to the impurity equation of state is fundamental in obtaining this peculiar effect.

Finally, as the magnetic field is further increased we show that for $B = 66.6\ G$ the impurity is localized at the center of the self-bound droplet

Let us consider just the effective potential V_{eff}, for a fixed droplet profile. Which states can it support?



a-b) Ground state of an impurity at $B = 66.6$ G and at $B = 65.8$ G.

c) Excited state of an impurity at $B = 65.8$ G for $\ell = 10$ and $m = 10$.

d) Effective potential $V_{\text{eff}}(r)$ and density of the impurity $n_I(r)$ for the $n = 0, \ldots, 3$ s-wave bound states.

e) Spectrum of the impurity eigenstates in the presence of the effective potential.

A new perspective: impurities on the surface of a sphere. Experimental realization via a bubble trap in microgravity (fall tower, ISS)?.

Conclusions and future perspectives

- In this work we studied the effect of an impurity in a two-component heteronuclear Bose mixture. Our findings provide access to relevant information for the study and the detection of Bose polarons in collisionally stable and long-lived Bose mixtures with important implications for further research.
- Interestingly, the surface and center bound states found in the droplet phase, occur in a range of magnetic fields where long-lived droplets have been already produced. In current experiments the existence of such states, in which the impurity either localizes in the center of the droplet or on its surface, could be probed by performing high-resolution imaging.
- Evaporation to zero temperature?

G. Bighin, A. Burchianti, F. Minardi, and T. Macrì, arXiv:2109.07451.

Thank you for your attention.

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