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

Giacomo Bighin

ICSM-ICQMT-2026, April 24th, 2026

Introduction: polarons 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.

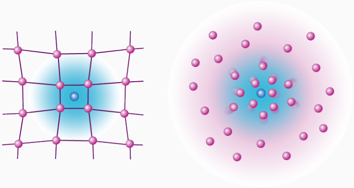

Image: APS/Carin Cain.

Introduction: polarons and Bose-Bose mixtures

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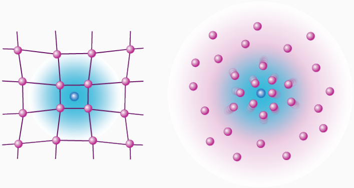

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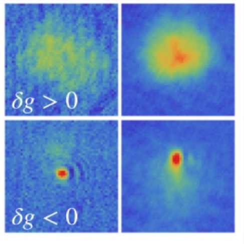


C. D'Errico *et al.*,
Phys. Rev. Research **1**, 033155 (2019).

A **Bose-Bose mixture** is an ultracold gas consisting of two different bosonic species. It has a very rich phase diagram including a remarkable self-bound **droplet state**: a quantum liquid. Quantum droplets have been observed recently, for instance in a **heteronuclear mixture of ^{41}K and ^{87}Rb**.

Interacting Bose-Bose mixture:

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

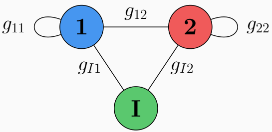
where $\hat{\phi}_i$, $\hat{\phi}_i^\dagger$ $(i = 1, 2)$ are bosonic field operators acting on two different bosonic species, m_i are the masses of each species and g_{ij} is the contact interaction strength between species i and species j.

Impurity in the mixture:

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

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

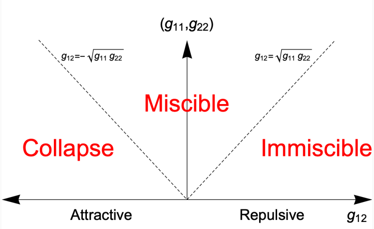
Many parameters: five different couplings!



Bose-Bose mixture: mean-field phase diagram

Mean-field description: one can obtain conditions for the stability of the mixture at $T = 0$ 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.



So far no trace of droplets or liquid-like behavior!

[1]See for instance C. Pethick and H. Smith, *"Bose-Einstein condensation in dilute gases"*, (Cambridge University Press, Cambridge, England, 2002).

What makes a liquid a liquid?

Image from: Wikimedia Commons

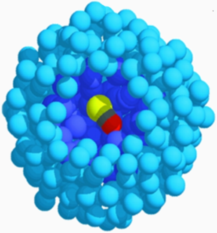


Image from: S. Grebenev, J.P. Toennies, A.F. Vilesov, Science **279**, 2083 (1998).

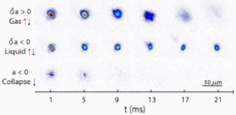


Image from: C.R. Cabrera *et al.*, Science **359**, 301 (2018).

Quantum liquids: self-bound quantum droplets

What makes a liquid a liquid?

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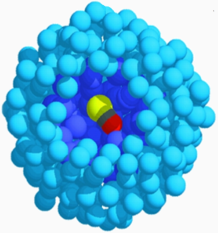

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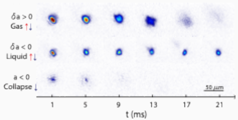

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Typically, it is a **balance** between repulsive and attractive interatomic forces!

Can this balance be engineered in ultracold matter?

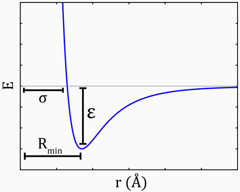

Image from: Wikibooks, *"Molecular simulation"*.

Beyond-mean-field stabilization of collapsing Bose-Bose mixture

Can **beyond-mean-field** effects alter this picture?

Beyond-mean-field stabilization of collapsing Bose-Bose mixture

Can **beyond-mean-field** effects alter this picture?

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, i.e. a quantum **liquid**.

✓ Beyond-mean-field effects completely alter the phase diagram! (Quantum fluctuation stabilization of BCC phase of He)

✓ Theoretical prediction in 2015, experimental observations starting from 2017.

PRL **115,** 155302 (2015) PHYSICAL REVIEW LETTERS week ending 9 OCTOBER 2015

Quantum Mechanical Stabilization of a Collapsing Bose-Bose Mixture

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(Received 28 June 2015; published 7 October 2015)

Self-bound quantum droplets in a Bose-Bose mixture

Single-component Bose gas

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

with the LHY correction accounting for quantum fluctuations on top of the Bogoliubov mean-field ground state. 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.

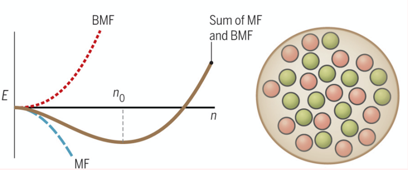
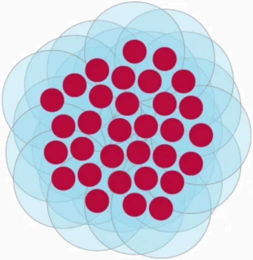


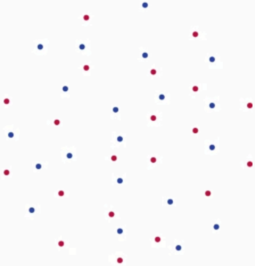
Image from: Science **359**, 274 (2018).

Self-bound quantum droplets in a Bose-Bose mixture

“Classical” van der Waals paradigm for a droplet: hard core + vdW tail



Quantum droplet: MF attraction + BMF repulsion



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

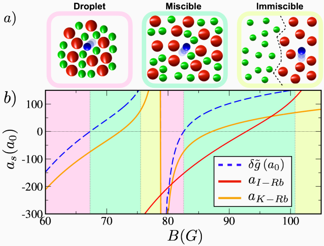
Images from D.S. Petrov, Nat. Phys. **14**, 211 (2018).

A closer look at the Bose-Bose mixture

We consider a specific experimental realization:

^{41}K — ^{87}Rb Bose mixture + ^{41}K impurity (different hyperfine state).

$a_{\text{I-Rb}}$, and $a_{\text{K-Rb}}$ are tunable with magnetic field via a Feshbach resonance; other scattering length are nearly constant $a_{\text{K-K}} \simeq a_{\text{I-K}} \simeq 62a_0$, $a_{\text{Rb-Rb}} \simeq 100.4a_0$, remember that $g = 4\pi\hbar^2 a/m$.



Scattering length calculations: A. Simoni.

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

GB, A. Burchianti, F. Minardi, T. Macrì, Phys. Rev. A **106**, 023301 (2022).

Theoretical framework: Bogoliubov approach to a Bose-Bose mixture

Generalization of **Bogoliubov treatment**[2]: expand the bosonic field in plane waves

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

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

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

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

$$\begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{a}^{\dagger}_{-\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \\ \hat{b}^{\dagger}_{-\mathbf{k}} \end{pmatrix}_i = \mathbb{M}^{-1}_{ij} \begin{pmatrix} \hat{A}_{\mathbf{k}} \\ \hat{A}^{\dagger}_{-\mathbf{k}} \\ \hat{B}_{\mathbf{k}} \\ \hat{B}^{\dagger}_{-\mathbf{k}} \end{pmatrix}_j$$

Result: the Hamiltonian is diagonal in the new field operators, but the impurity now couples to hybrid normal modes, not to physical species.

Analogous to acoustic and optical branches in a **two-sublattice phonon problem**: two-band superconductors exhibiting a density and a spin mode.

[2] D. M. Larsen, Annals of Physics **24**, 89 (1963).

Miscible phase: Hamiltonian

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

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

It has been shown[3] 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**

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

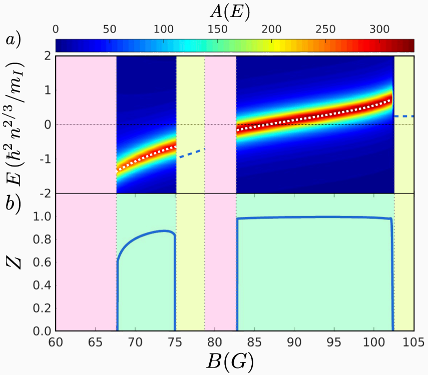
having grouped the creation and annihilation operators into a spinor-like object $\Psi(\mathbf{k}) = (a_{\mathbf{k}}\ a^\dagger_{-\mathbf{k}}\ b_{\mathbf{k}}\ b^\dagger_{-\mathbf{k}})^T$.

[3] 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 $92.8\ G$.

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 single complex field $\phi(\mathbf{r})$ with the associated energy functional

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

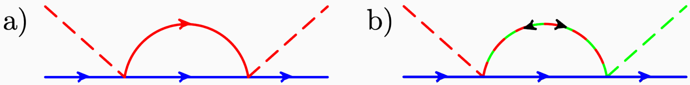
where the last term is the beyond mean-field interaction for a general two-component mixture. The **impurity interaction** with the Bose mixture is described by the energy functional

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

The last term $\mathscr{E}_{\text{BMF}}(\mathbf{r})$ is the **beyond-mean-field interaction** for a general two-component mixture. Note that $\mathscr{E}_{\text{BMF}} \propto n^{3/2}$.

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[4]. **Novel feature**: diagrams mixing different normal components of the condensate.



The **energy correction** $\mathscr{E}_{\mathsf{BMF}}$ 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.

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

Droplet phase: Gross-Pitaevskii equations

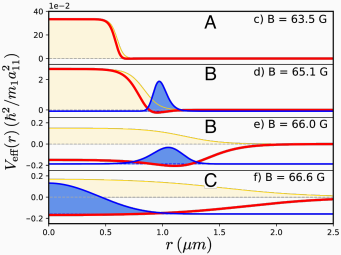
We finally obtain the (rescaled) **Gross-Pitaevskii equations** to be solved numerically for the impurity-droplet system (the impurity has mass m_1)

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

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

Droplet phase: three different impurity regimes

We study the effect of an impurity in the droplet phase within the Gross-Pitaevskii framework. Rich phenomenology, three different regimes.



Effective potential seen by the impurity:

$$V_{\text{eff}}(\mathbf{r}) = g_{ID}|\phi(\mathbf{r})|^2 + \mathscr{E}_{\text{BMF}}(\mathbf{r})$$

Regime A: 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.

Regime B: for $B = 65.1\ G$ and for $B = 66.0\ G$ the impurity is localized at the surface of the droplet at a distance $r \approx 1 \mu m$ form the center.

Regime C: for $B = 66.6\ G$ the impurity is localized at the center of the self-bound droplet.

GB, A. Burchianti, F. Minardi, T. Macrì, Phys. Rev. A **106**, 023301 (2022).

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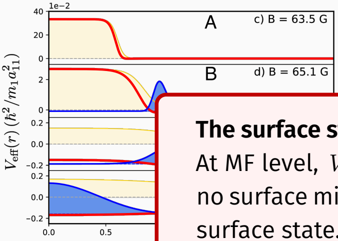

Effective potential seen by the impurity:

$$V_{\text{eff}}(\mathbf{r}) = g_{ID}|\phi(\mathbf{r})|^2 + \mathscr{E}_{\text{BMF}}(\mathbf{r})$$

The surface state has no mean-field counterpart. At MF level, $V_{\text{eff}} \propto |\phi|^2$ is monotonic in density — no surface minimum. It is $\mathscr{E}_{\text{BMF}}$ that **generates** the surface state.

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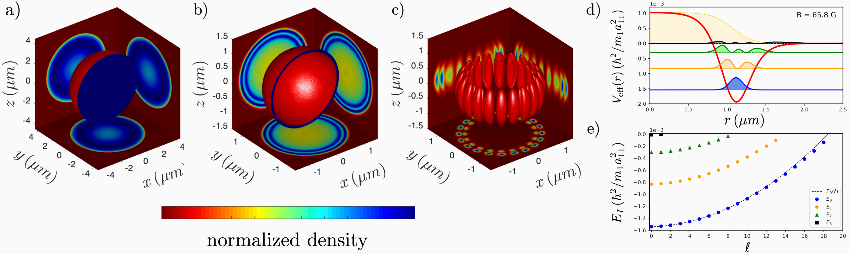
Rotational states: an impurity on the surface of a sphere?

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.

Current work and future perspective

- Effective low-energy Hamiltonian for of an impurity on a sphere.
- More than one impurity: effective **bath-mediated interaction**.
- Impurities on the surface of a sphere with **repulsive interaction**: appearance of **Wigner crystalization**.

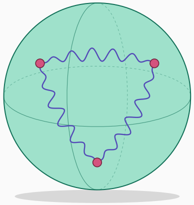


Image credit: Claude AI

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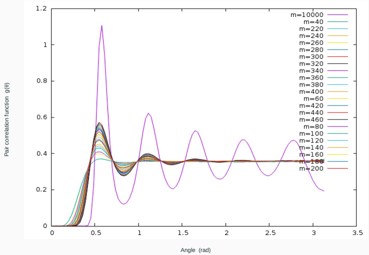

Angular pair correlation function of repulsive particles on a sphere: crystallization.

Conclusions and future perspectives

- In this work we studied and characterized an impurity in a two-component heteronuclear Bose mixture, paving the way for the study and the detection of Bose polarons in collisionally stable and long-lived Bose mixtures.
- Quantum droplets can host distinct impurity phases — **center-bound** and **surface-bound** states — that should be directly observable with current high-resolution imaging in experimentally accessible regimes.
- **Dopant spectroscopy** provides a direct window into droplet properties, offering a route toward quantitative characterization and potentially access to the near-zero-temperature regime. Evaporation to zero temperature?

G. Bighin, A. Burchianti, F. Minardi, and T. Macrì, Phys. Rev. A **106**, 023301 (2022).

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G. Bighin, A. B… 01 (2022).

In collaboration with:

Alessia Burchianti – LENS, Florence

Francesco Minardi – Bologna

Tommaso Macrì – now at QuEra Computing

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These slides at http://bigh.in

Backup slide # 1

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) \approx \prod_{i=1}^{N} \phi(\mathbf{r}_i, t) \quad (1)$$

Backup slide # 2

Backup slide # 3