The 23rd International Conference on
Few-Body Problems in Physics (FB23)

# Microwave Shielded Polar Molecules

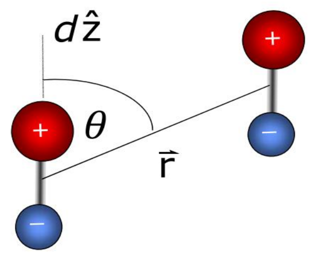
Tao Shi

*23rd Sep. 2024, Beijing, China*

PRL **130**, 183001 (2023); Nature **626**, 283 (2024);
arXiv:2405.13645; arXiv:2406.06412

# Dipolar interactions

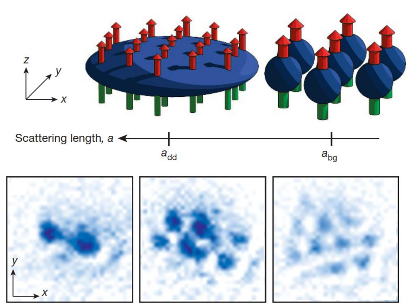
***Dipolar interaction: long-range and anisotropic***




$$U_\mathrm{d}(\vec{r}) = \frac{d^2}{4\pi\epsilon_0}\frac{1-3\cos^2\theta}{r^3}$$

### *Magnetic Atoms*

*Weak dipoles ~ 10 $\mu_B$, stable (10 s)*

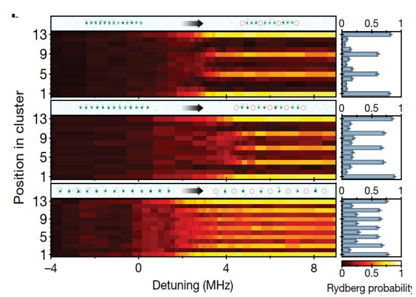



H. Kadau et al.,

Nature 530, 194 (2016)

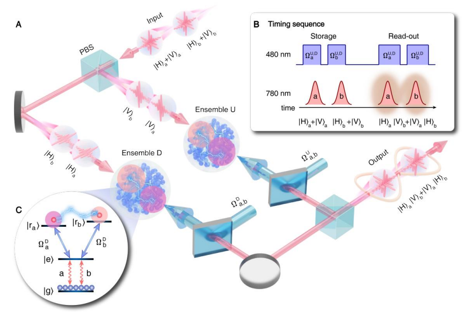
### *Rydberg Atoms*

*Strong dipoles ~ 104 Debye, lifetime ~ 100 μs*




H. Bernien et al.,

Nature 551, 579 (2017)

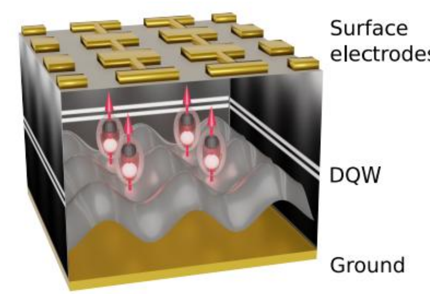



G. Ye, et al.,

Nature Photonics (2023)

### *Dipolar Excitons*

*Strong dipoles ~ 103 Debye, lifetime ~ 1 μs*

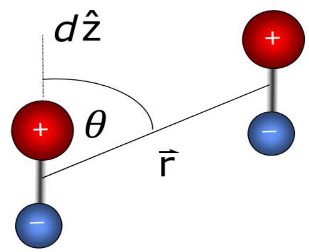



C. Lagoin et al.,

Nature 609, 485 (2022)

# Dipolar interactions

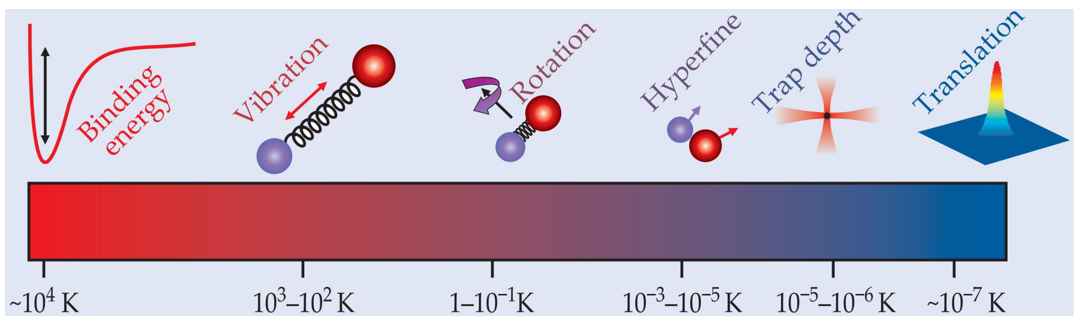
***Dipolar interaction: long-range and anisotropic***




$$U_{\mathrm{d}}(\vec{r}) = \frac{d^2}{4\pi\epsilon_0}\frac{1-3\cos^2\theta}{r^3}$$

## ***Dipolar Molecules***

*Medium dipoles ~ 3 Debye, alone stable (10 s)*

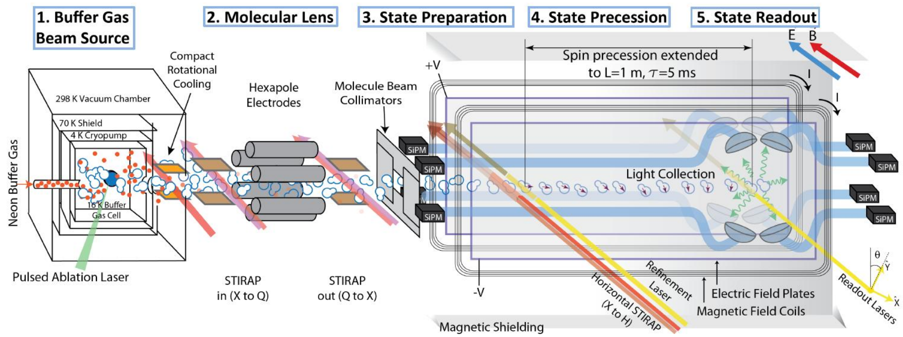



Jin & Ye Physics Today 64, 5, 27 (2011)

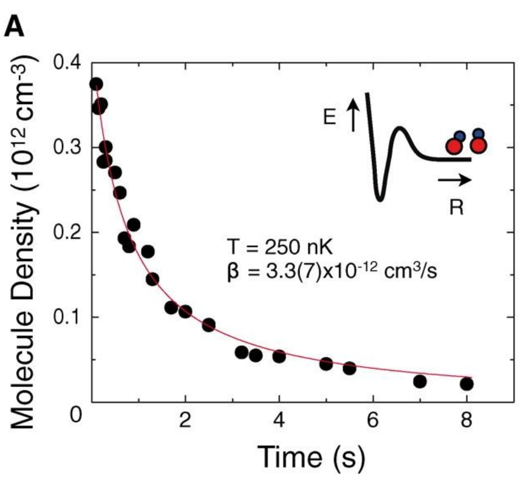
# Polar Molecules

## *Precision measurement*

ACME III (Harvard),JILA, ICL, Caltech, Amsterdam…



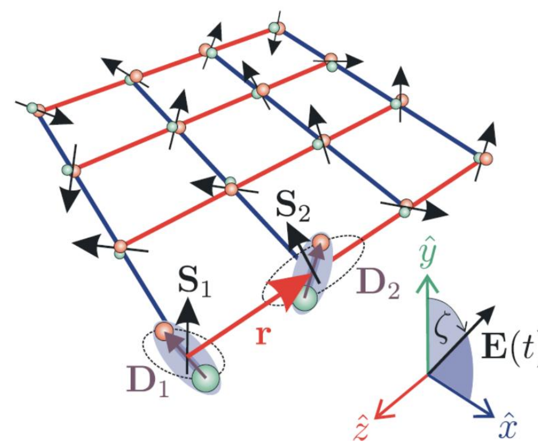

## *Ultracold chemistry*




$$KRb + KRb \rightarrow K_2 + Rb_2$$

JILA, 2010

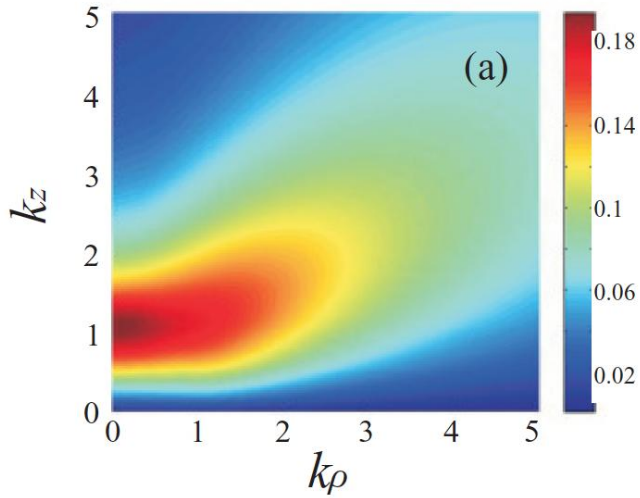
## *Spin systems*



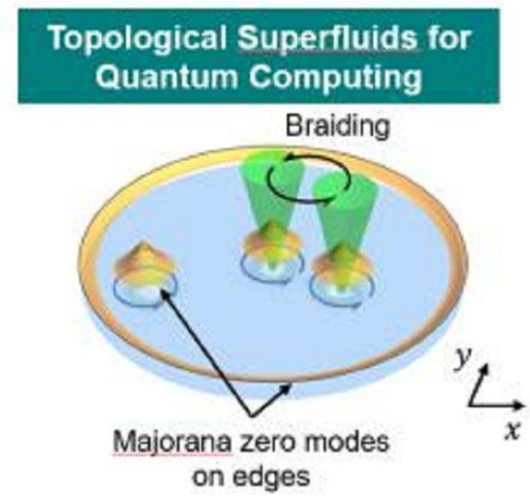

A. Micheli, Nat. Phys. 2, 341 (2006).

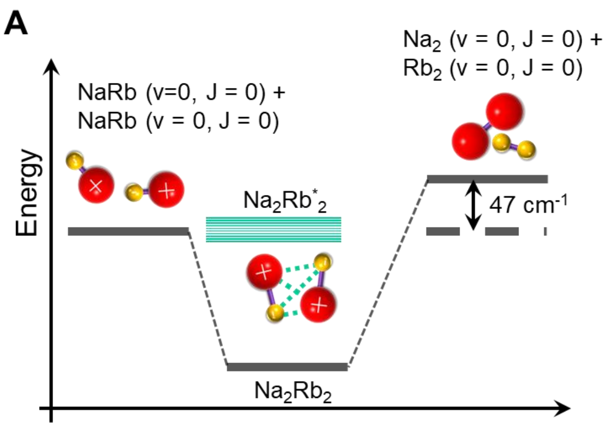
# BCS-BEC in Polar Molecules

***Dipolar superfluids***



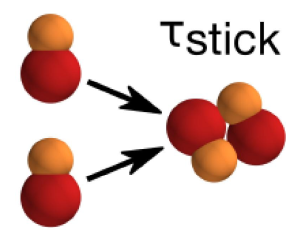

You and Marinescu, PRA 60, 2324 (1999).
Baranov et al., PRA 66, 013606 (2002).
Cooper and Shlyapnikov, PRL 103, 155302 (2009).
Shi, Zhang, Sun, and Yi, PRA **82**, 033623 (2010).
Wu and Hirsch, PRB **81**, 020508 (2010).
Shi, Zou, Hu, Sun, and Yi, PRL 110, 045301 (2013).
Qi, Shi, and Zhai, PRL 110, 045302 (2013).




X. Ye, et al., Sci. Adv. 4, eaaq0083 (2018).

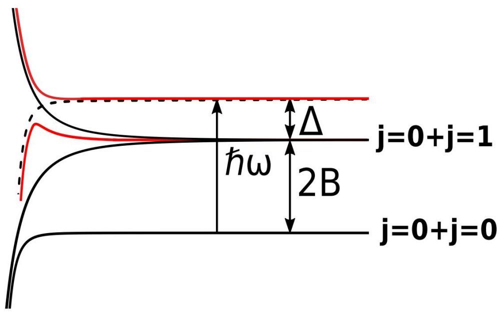
***unstable at the short range***




Bause et al., PRR 3, 033013 (2021).

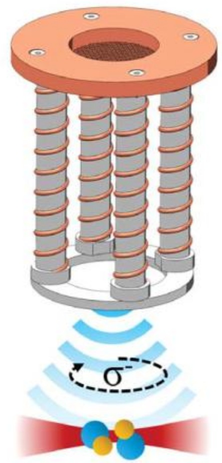
# Microwave Shielding

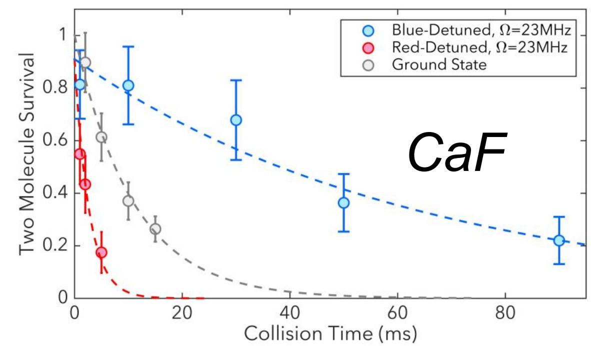
***Theoretical proposal:***




Karman and Hutson, PRL 121, 163401 (2018)
Lassablière and Quéméner, PRL 121, 163402 (2018)

***Suppression of inelastic scatterings:***




Anderegg et al., Science 373, 779 (2021).

# Realization of fermionic MSPMs

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Andreas Schindewolf, Roman Bause, Xing-Yan Chen, Marcel Duda, Tijs Karman, Immanuel Bloch & Xin-Yu Luo ✉

*Nature* **607**, 677–681 (2022) | Cite this article

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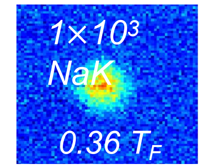


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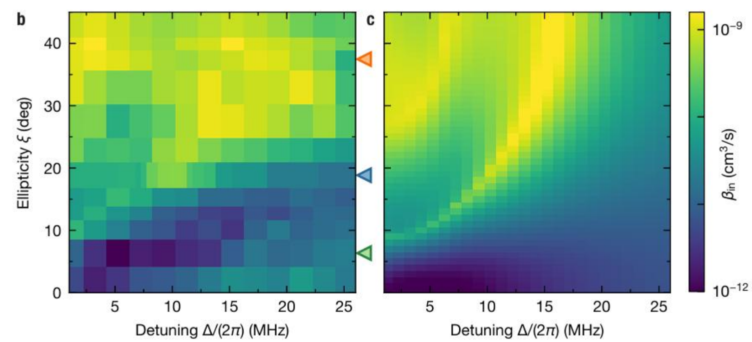


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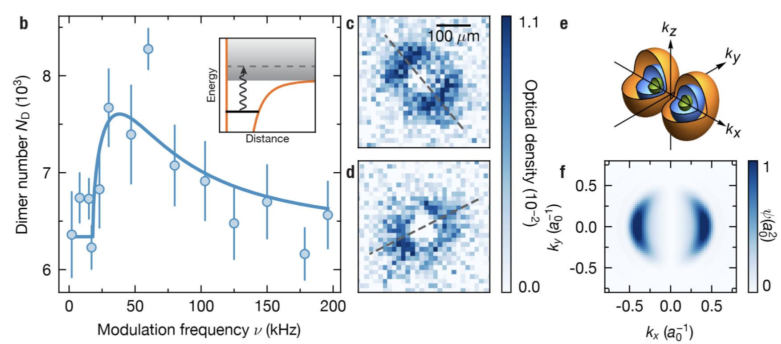
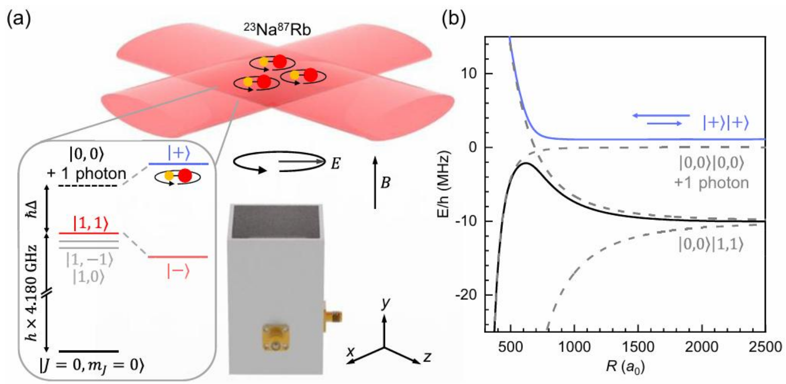
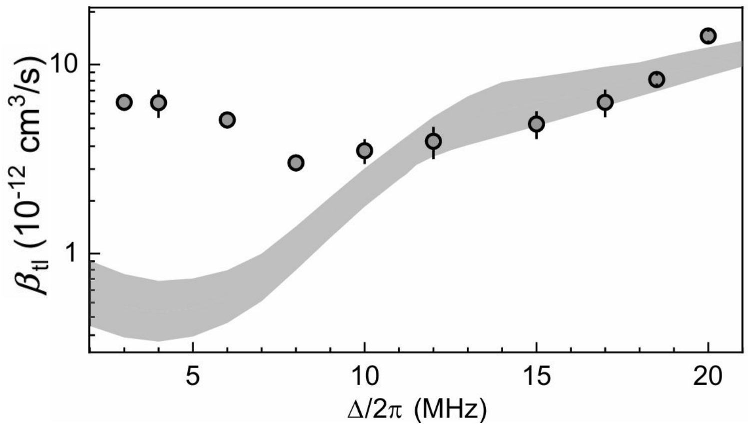


# Realization of Bosonic MSPMs




J. Lin et al., Phys. Rev. X **13**, 031032 (2023)

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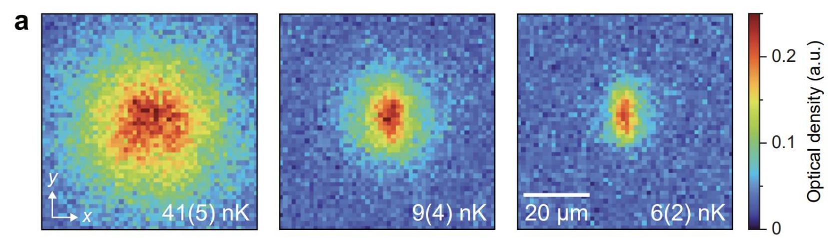
**Observation of Bose–Einstein condensation of dipolar molecules**

Niccolò Bigagli, Weijun Yuan, Siwei Zhang, Boris Bulatovic, Tijs Karman, Ian Stevenson & Sebastian Will

*Nature* **631**, 289–293 (2024) | Cite this article



# Outline

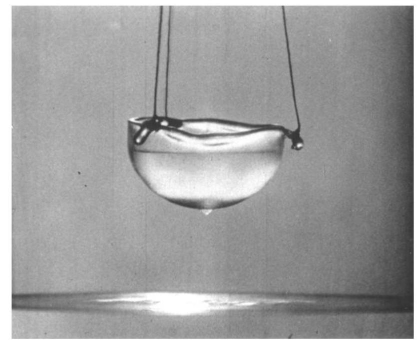
Introduction

Effective potentials for MSPMs

Fermionic MSPMs

Bosonic MSPMs

Conclusion and Outlook

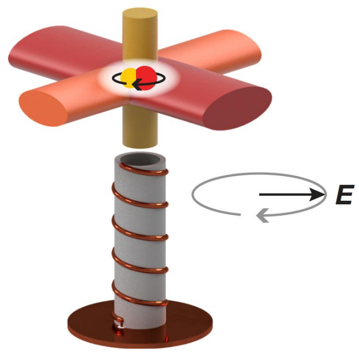


Liquid Helium

Effective potentials for MSPMs

# Microwave shielding

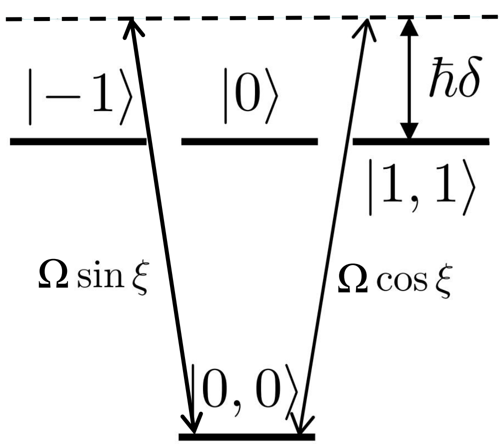
***Single molecule:***

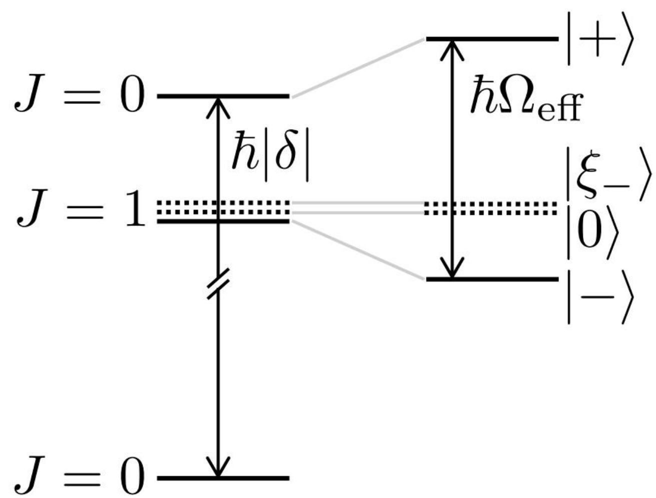



$$\frac{\hbar\Omega}{2} e^{-i\omega_0 t} |\xi_+\rangle\langle 0,0| + \text{h.c.}$$

$$|\xi_+\rangle \equiv \cos\xi\,|1,1\rangle + \sin\xi\,|1,-1\rangle$$

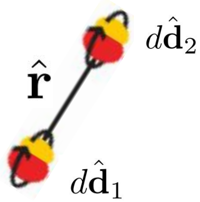
$$|\xi_-\rangle \equiv \cos\xi\,|1,-1\rangle - \sin\xi\,|1,1\rangle$$



# Microwave shielding

***Two molecules:***




Two-body Hamiltonian:

$$\hat{H}_2 = \sum_{j=1,2} \hat{h}_j + V(\mathbf{r}_1 - \mathbf{r}_2)$$

Kinetic energy:

$$\hat{h}_j = -\hbar^2 \nabla_j^2/(2M) + \hat{h}_{\rm in}(j)$$

# Microwave shielding

***Two molecules:***


Two-body Hamiltonian:

$$\hat{H}_2 = \sum_{j=1,2} \hat{h}_j + \boxed{V(\mathbf{r}_1 - \mathbf{r}_2)}$$

Kinetic energy:

$$\hat{h}_j = -\hbar^2 \nabla_j^2/(2M) + \hat{h}_{\text{in}}(j)$$

Dipolar interaction:

$$V(\mathbf{r}) = \frac{d^2}{4\pi\epsilon_0 r^3}\left[\hat{\mathbf{d}}_1 \cdot \hat{\mathbf{d}}_2 - 3(\hat{\mathbf{d}}_1 \cdot \hat{\mathbf{r}})(\hat{\mathbf{d}}_2 \cdot \hat{\mathbf{r}})\right]$$

$$= -8\sqrt{\frac{2}{15}}\pi^{3/2}\frac{d^2}{4\pi\epsilon_0 r^3}\sum_{m=-2}^{2} Y_{2m}^*(\hat{\mathbf{r}})\Sigma_{2,m},$$

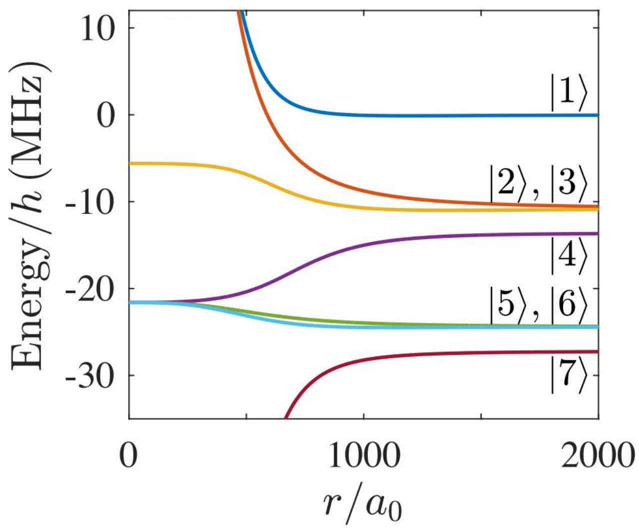
Spherical tensors:

$$\Sigma_{2,0} = \frac{1}{\sqrt{6}}(\hat{d}_1^+\hat{d}_2^- + \hat{d}_1^-\hat{d}_2^+ + 2\hat{d}_1^0\hat{d}_2^0),\ \Sigma_{2,\pm1} = \frac{1}{\sqrt{2}}(\hat{d}_1^\pm\hat{d}_2^0 + \hat{d}_1^0\hat{d}_2^\pm),\ \text{and}\ \Sigma_{2,\pm2} = \hat{d}_1^\pm\hat{d}_2^\pm$$

The parity symmetry reduces the Hamiltonian to a 7D matrix in the symmetric space.

# Microwave shielding

***BO approximation:***




$$|1\rangle = |+,+\rangle,$$

$$|2\rangle = |+,0\rangle_s,\ |3\rangle = |+,\xi_-\rangle_s,$$

$$|4\rangle = |+,-\rangle_s,$$

$$|5\rangle = |-,0\rangle_s,\ |6\rangle = |-,\xi_-\rangle_s,$$

$$|7\rangle = |-,-\rangle$$

$|1\rangle$ mostly couples to $|\mathrm{c}\rangle = \frac{1}{\sqrt{\cos^2\theta + 1}}(\sqrt{2}\cos\theta\,|2\rangle_{\mathrm{s}} + \sin\theta e^{i\varphi}\,|3\rangle_{\mathrm{s}}).$

The 7D Hamiltonian is further reduced to a 2D matrix, which can be solved analytically!

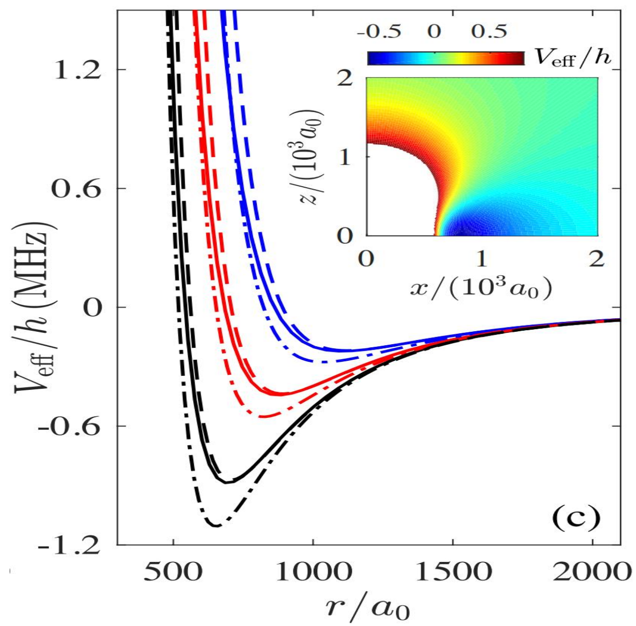
# Microwave shielding

***Effective potential:***

$$V_{\text{eff}}(\mathbf{r}) = \frac{C_3}{r^3}[3\cos^2\theta - 1 + 3\mathcal{F}_\xi(\varphi)\sin^2\theta] + \frac{C_6}{r^6}\sin^2\theta\{1-\mathcal{F}_\xi^2(\varphi)+[1-\mathcal{F}_\xi(\varphi)]^2\cos^2\theta\}.$$

$$\mathcal{F}(\xi,\varphi) \;=\; \sin 2\xi\cos 2\varphi$$

$$C_3 = d^2/\left[48\pi\epsilon_0(1+\delta_r^2)\right] \qquad C_6 = d^4/\left[128\pi^2\epsilon_0^2\Omega(1+\delta_r^2)^{3/2}\right]$$




F.Deng, X. Y. Chen, X. Y. Luo, W. Zhang, S. Yi, and TS, PRL 130, 183001 (2023)

# Algorithm

## *7-Channel Scatterings:*

$$\sum_{\nu'=1}^{7}\left(-\frac{\hbar^2\nabla^2}{M}\delta_{\nu\nu'}+V_{\nu\nu'}\right)\psi_{\nu'}(\mathbf{r})=\frac{\hbar^2k_\nu^2}{M}\psi_\nu(\mathbf{r}),$$

Angular momentum basis:

$$\psi_\nu(\mathbf{r}) \;=\; \sum_{lm} Y_{lm}(\hat{\mathbf{r}})\phi_{\nu lm}(r)/r$$

Log-derivative method:

B. Johnson, Journal of Computational Physics 13, 445 (1973).

$$\partial_r\mathcal{Y}(r)=-\mathcal{V}(r)-\mathcal{Y}^2(r) \qquad \mathcal{Y}(r)=\partial_r\phi(r)\phi^{-1}(r)$$

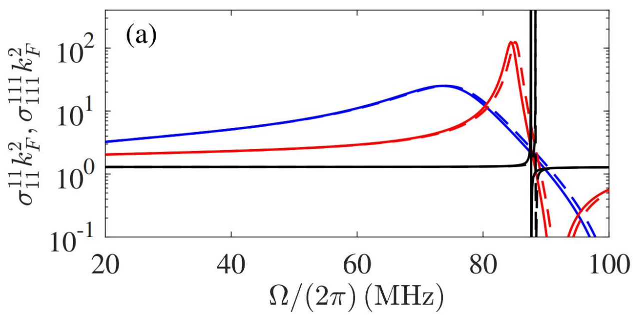
Matching the asymptotic solution:

$$\phi^{\mathrm{a}}_{\nu'l'm',\nu lm}(r)=\mathbf{J}_l(k_\nu r)\delta_{\nu\nu'}\delta_{ll'}\delta_{mm'}+\mathbf{N}_{l'}(k_{\nu'}r)\boxed{K_{\nu'l'm',\nu lm},}$$

$$f_{\nu lm}^{\nu'l'm'}=i\frac{1}{\sqrt{k_{\nu'}}}\left(\frac{1}{K+i}K\right)_{\nu'l'm',\nu lm}\frac{1}{\sqrt{k_\nu}} \qquad \sigma_{\nu lm}^{\nu'l'm'}=4\pi\left|f_{\nu lm}^{\nu'l'm'}\right|^2$$

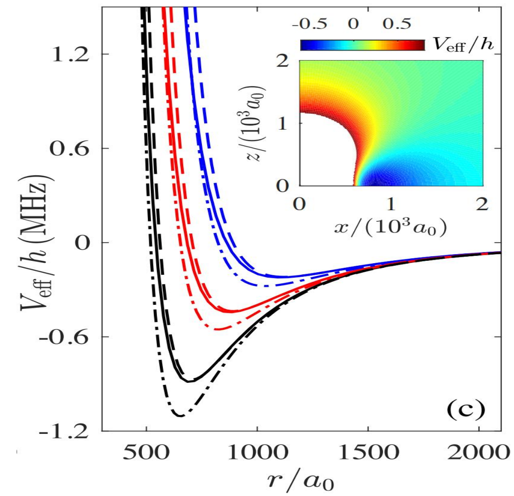
# Scattering cross sections

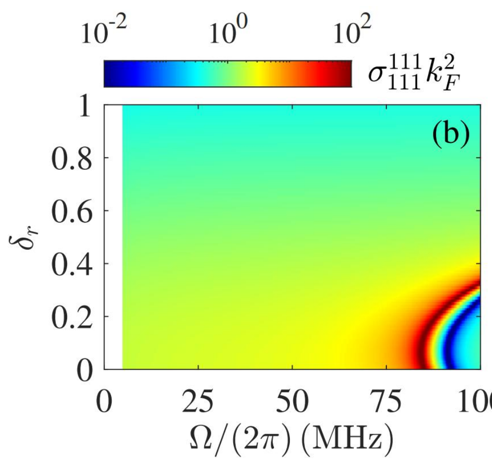
***p*-wave:**

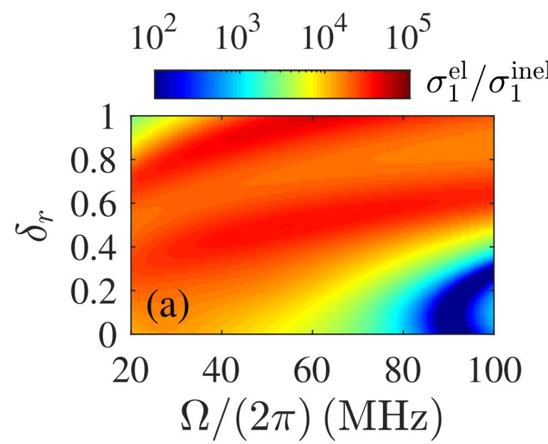



$k_1/k_F = 0.04$ (black lines),

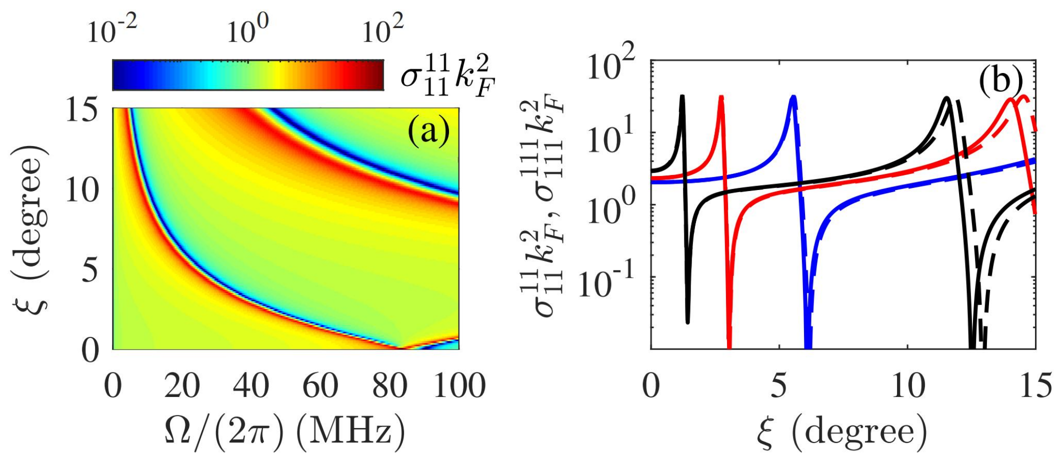
0.45 (red lines), and 1 (blue lines).

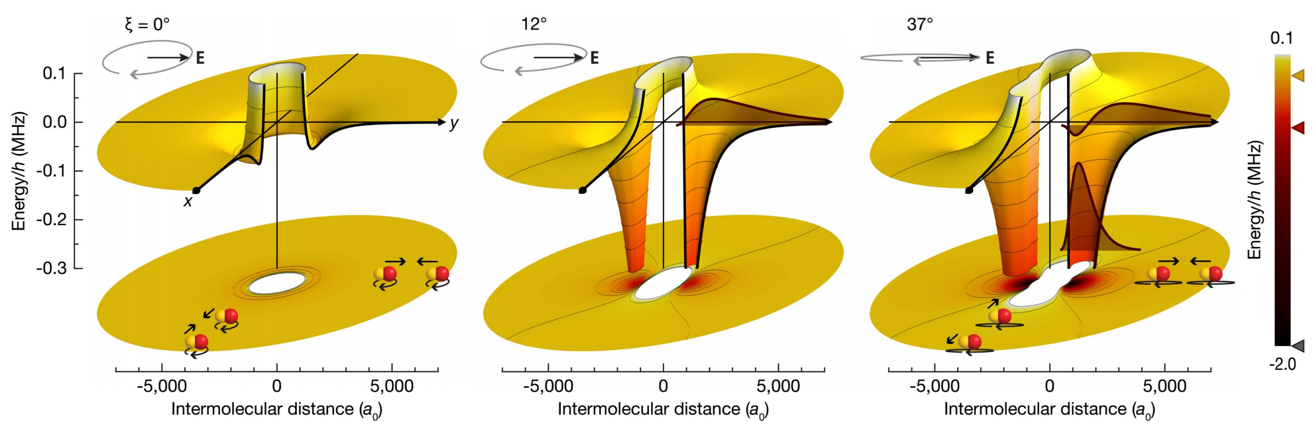


# Finite elliptic angles

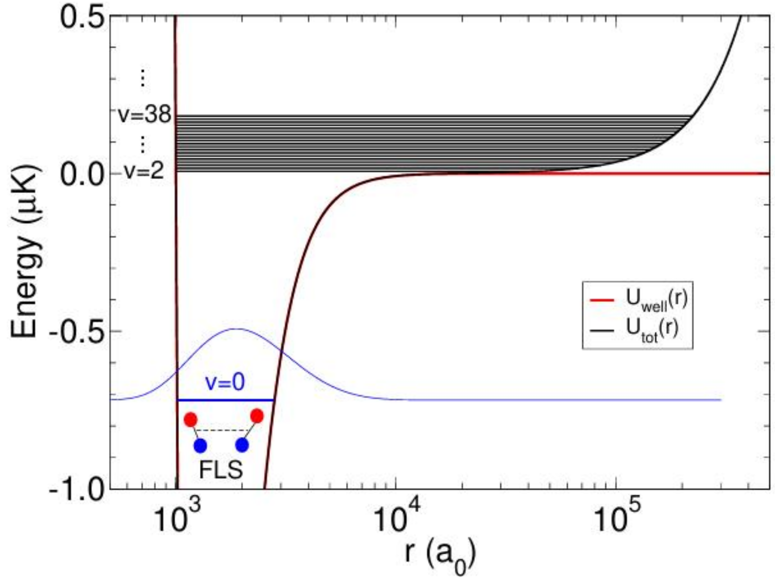


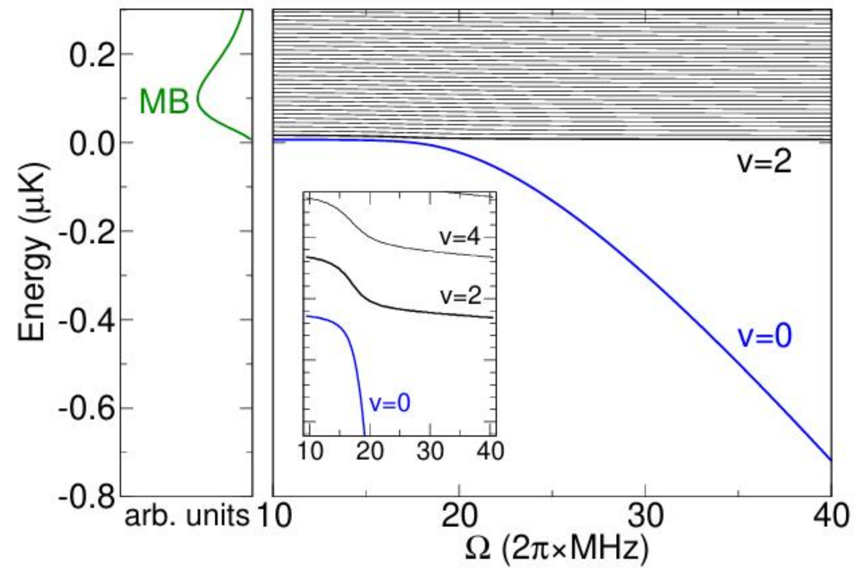




$$V_{\text{eff}}(\mathbf{r}) \sim -C_3(1+3\sin 2\xi)/r^3$$

X. Y. Chen, et al., Nature **614**, 59 (2023)

# Tetramer bound states

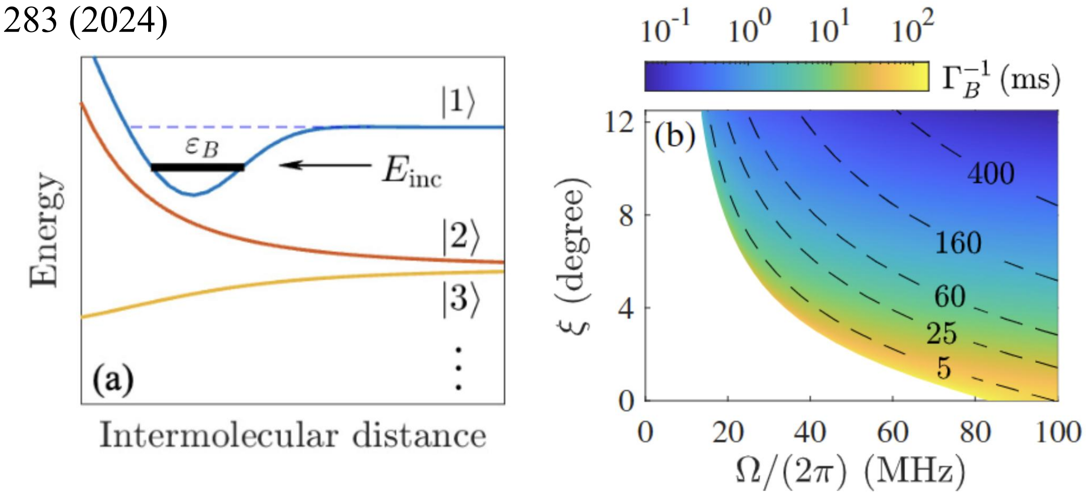


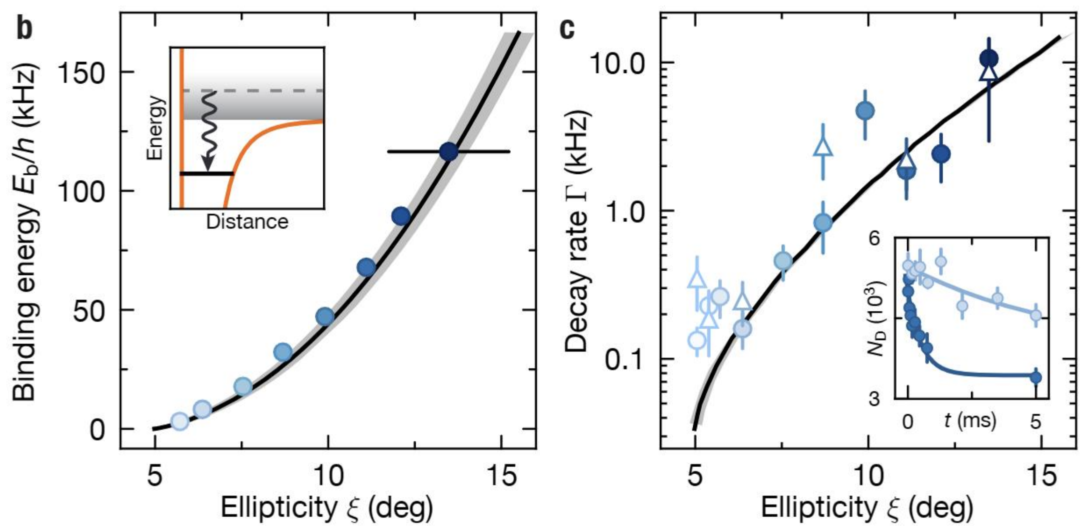

Goulven Quéméner, John L. Bohn, and James F. E. Croft,
Phys. Rev. Lett. **131**, 043402 (2023)

# Tetramer bound states

X. Y. Chen et al., Nature **626**, 283 (2024)



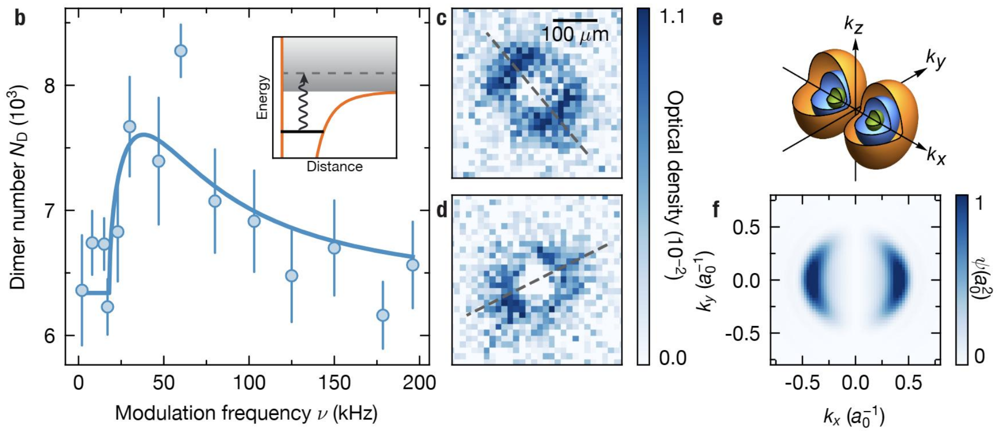

$$\sigma(E_{\text{inc}}) = \frac{2\pi}{k_2^2}\left|ig^2 G(E_{\text{inc}}) + S_{\text{bg}} - 1\right|^2$$

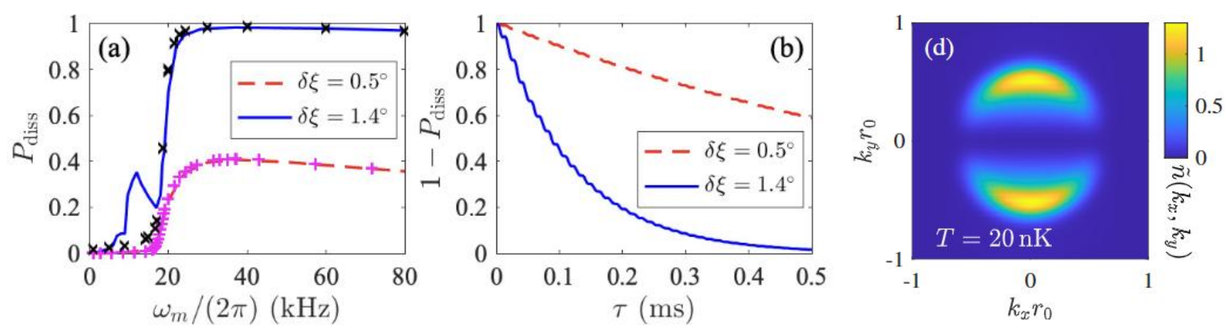


# Modulational dissociation

$$V_{\rm eff}(\mathbf{r}) = \frac{C_3}{r^3}[3\cos^2\theta - 1 + 3\mathcal{F}_\xi(\varphi)\sin^2\theta] + \frac{C_6}{r^6}\sin^2\theta\{1 - \mathcal{F}_\xi^2(\varphi) + [1-\mathcal{F}_\xi(\varphi)]^2\cos^2\theta\}.$$

$$H_{\rm MD} \approx (\varepsilon_B + \omega_{\rm m})\,|\psi_B\rangle\langle\psi_B| + \int d\mathbf{k}\frac{k^2}{M}|\psi_\mathbf{k}\rangle\langle\psi_\mathbf{k}| + \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} g_\mathbf{k}\,|\psi_\mathbf{k}\rangle\langle\psi_B| + \text{h.c.},$$



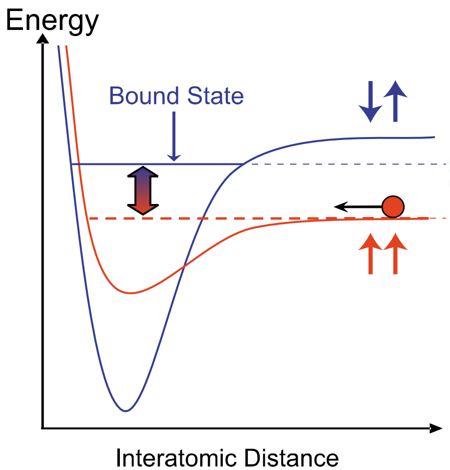



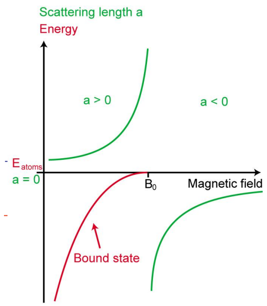


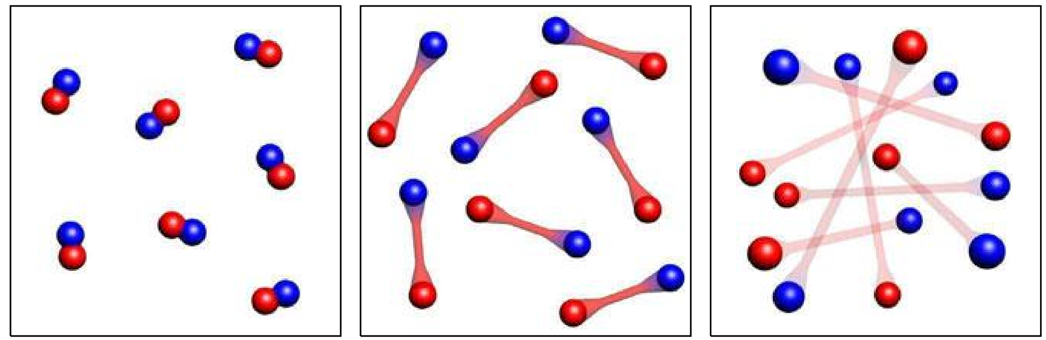
X. Y. Chen et al., Nature 626, 283 (2024)
F. Deng *et al.*, arXiv:2405.13645

# Fermionic MSPMs

# BCS-BEC crossover in atomic gases

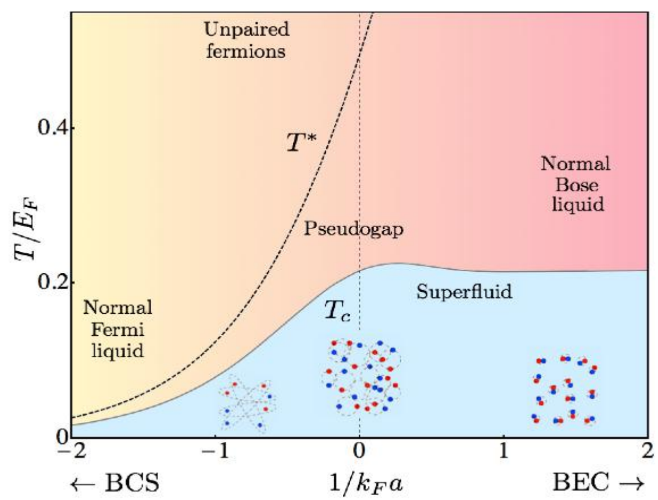


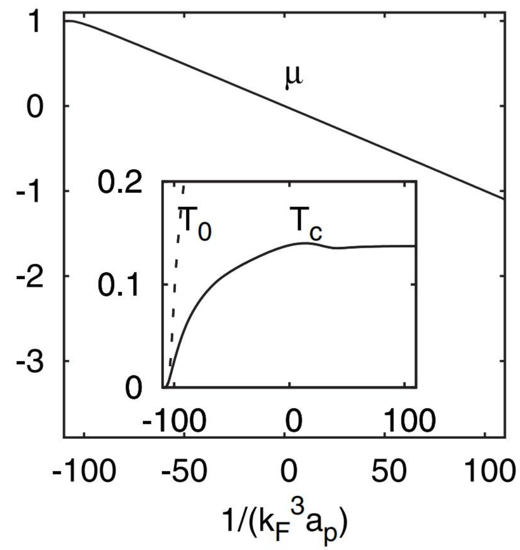



BEC of Molecules | Crossover Superfluid | BCS state

s-wave



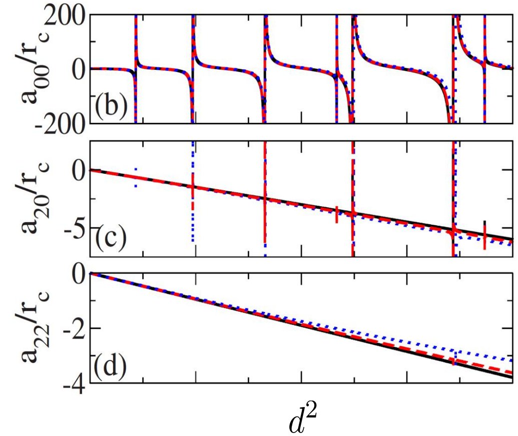

p-wave



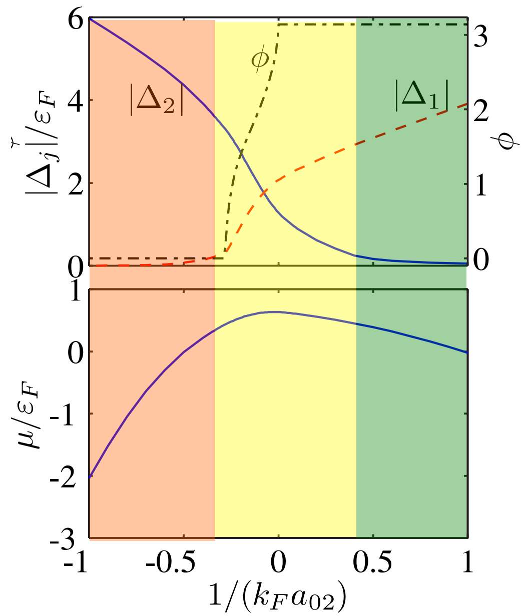

Sa de Melo et al., PRL **71**, 3283 (1993); PRL **96**, 040402 (2006).

# BCS-BEC crossover in dipolar gases

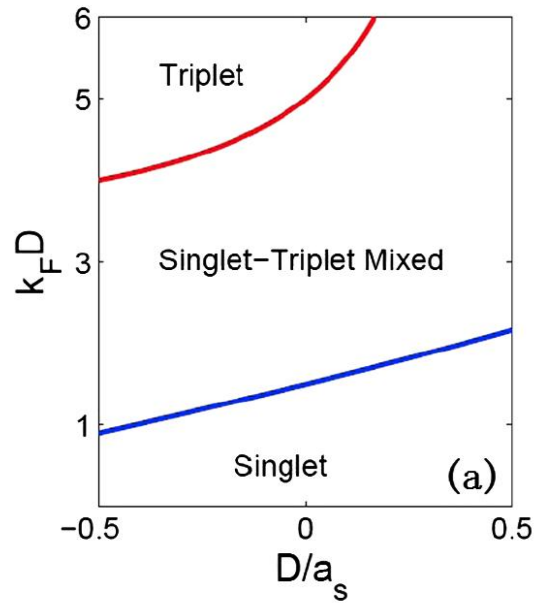
$$-\frac{M\Delta_j}{16\pi^2\lambda_j} = \sum_{j'} \Delta_{j'} \int \frac{d^3p}{(2\pi)^3} W_j^*(\hat{\mathbf{p}}) \left( \frac{1}{2E_{\mathbf{p}}} - \frac{M}{p^2} \right) W_{j'}(\hat{\mathbf{p}})$$




Kanjilal and Blume, PRA 78, 040703(R) (2008)




Shi, Zou, Hu, Sun, & Yi, PRL 110, 045301 (2013).




Qi, Shi, and Zhai, PRL 110, 045302 (2013).

# BCS superfluid in MS molecules

***Many-body Hamiltonian:***

$$\hat{H} = \int d^3\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2M} - \mu\right)\hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V_{\text{eff}}(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}),$$

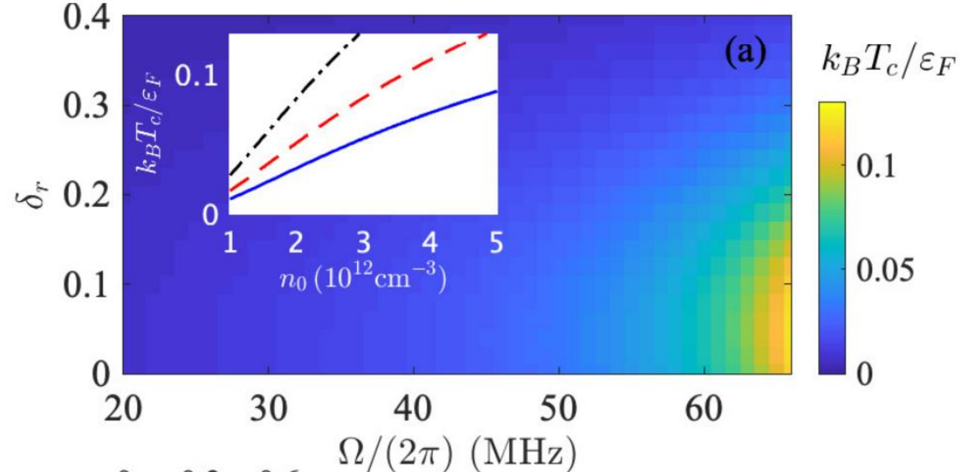
***Gap equation:***

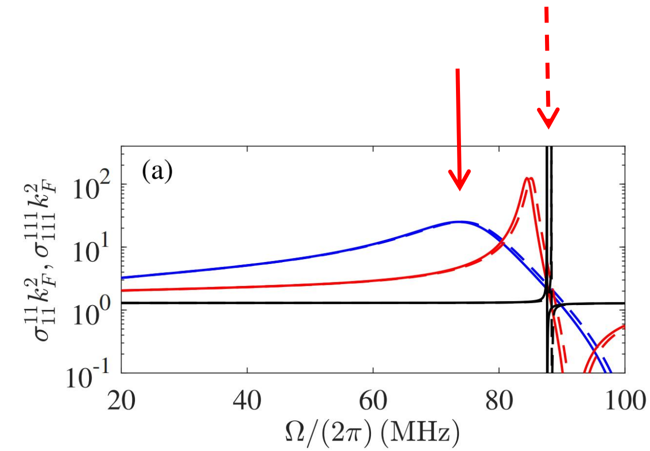
$$\Delta_{lm}(k) = -\frac{2}{\pi}\sum_{l'} i^{l'-l}\int_0^\infty p^2 dp \boxed{\widetilde{V}_{ll',m}(k,p)} \frac{\tanh(\beta_c\varepsilon_{\mathbf{p}}/2)}{2\varepsilon_{\mathbf{p}}}\Delta_{l'm}(p)$$

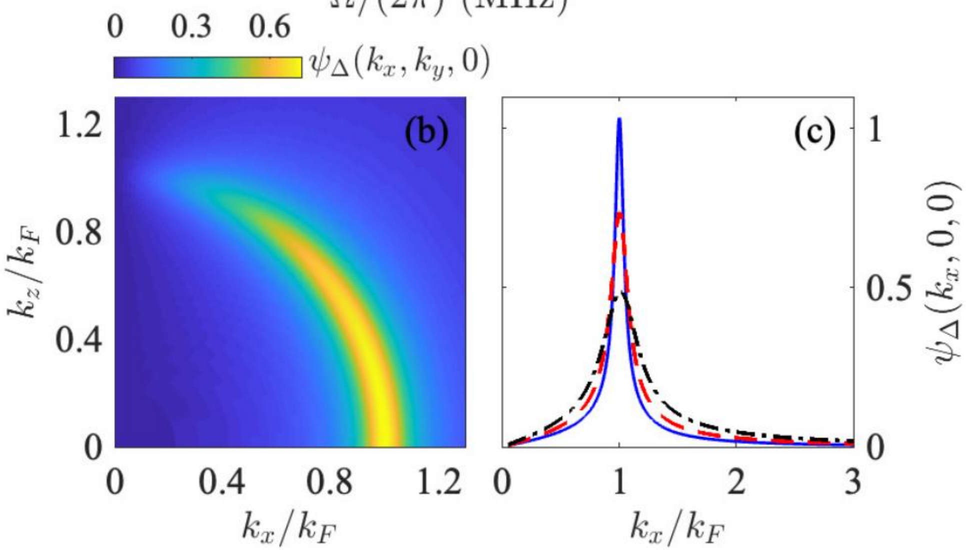
(1) Renormalization free
(2) Logrithmic discretization

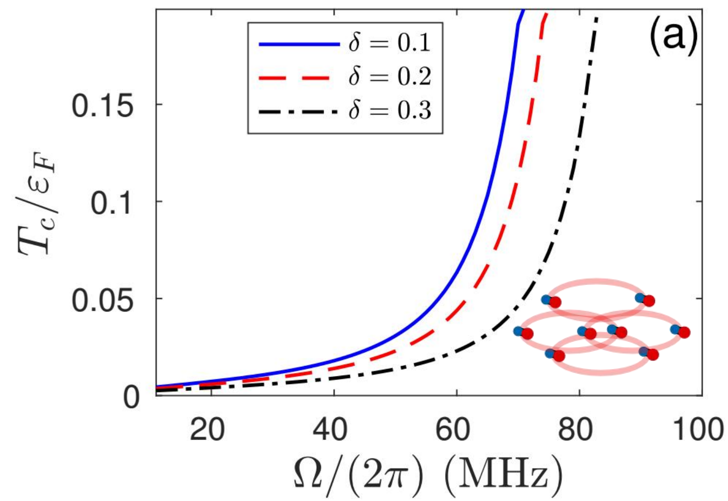
# BCS superfluid in MS molecules

$\Omega/(2\pi) = 28$ (solid line), 38 (dashed line), and 48 MHz (dash-dotted line)



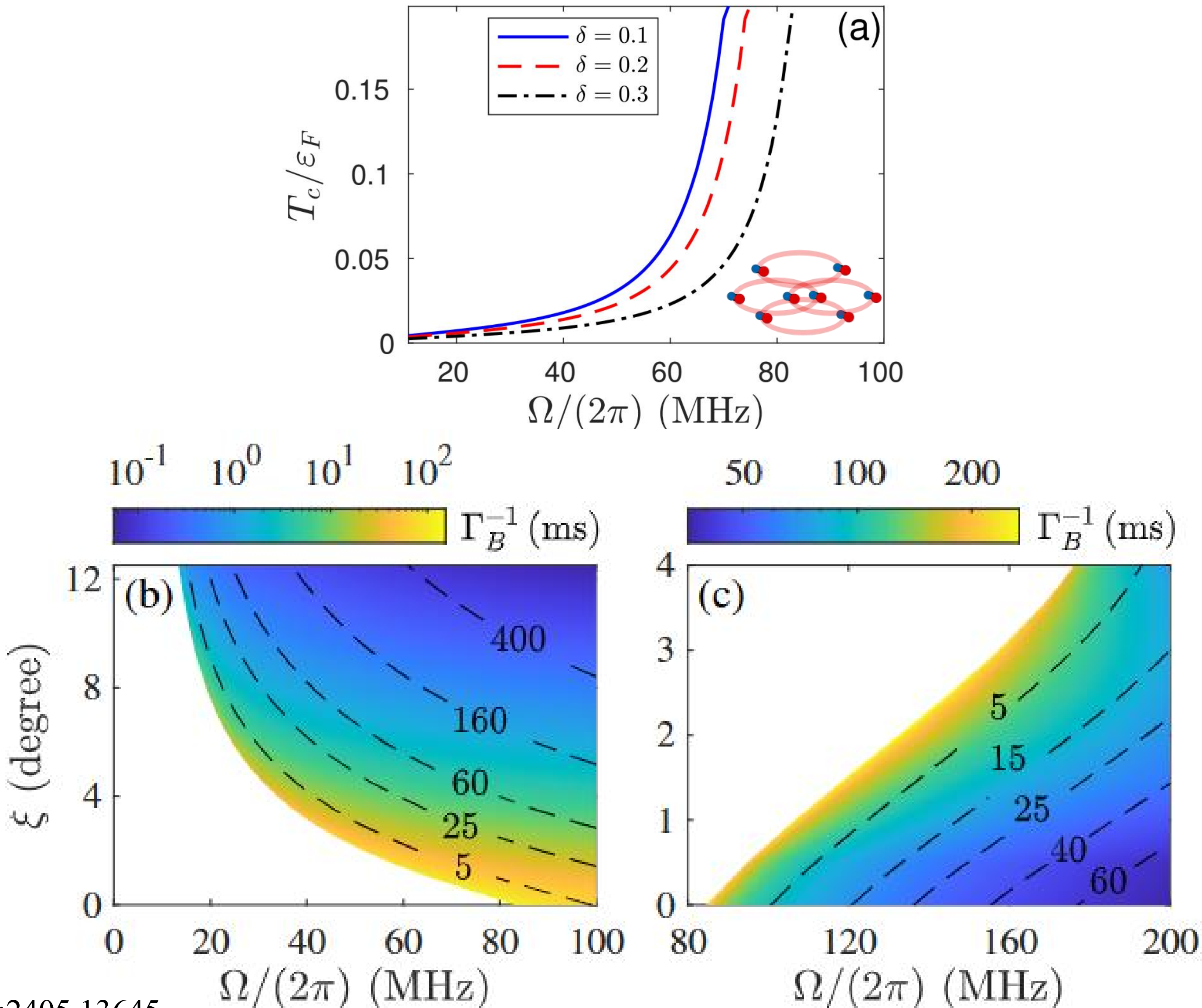




$\Omega/(2\pi) = 48$ (solid line), 58 (dashed line), and 66 MHz (dash-dotted line)

# Extending lifetimes of tetramers

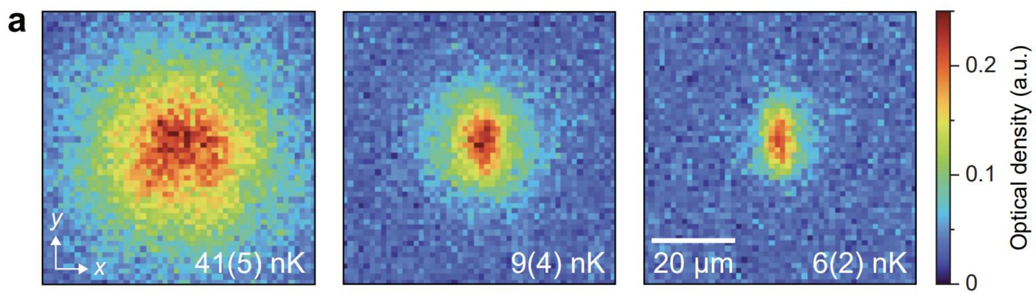



***LiRb: 10.4s***

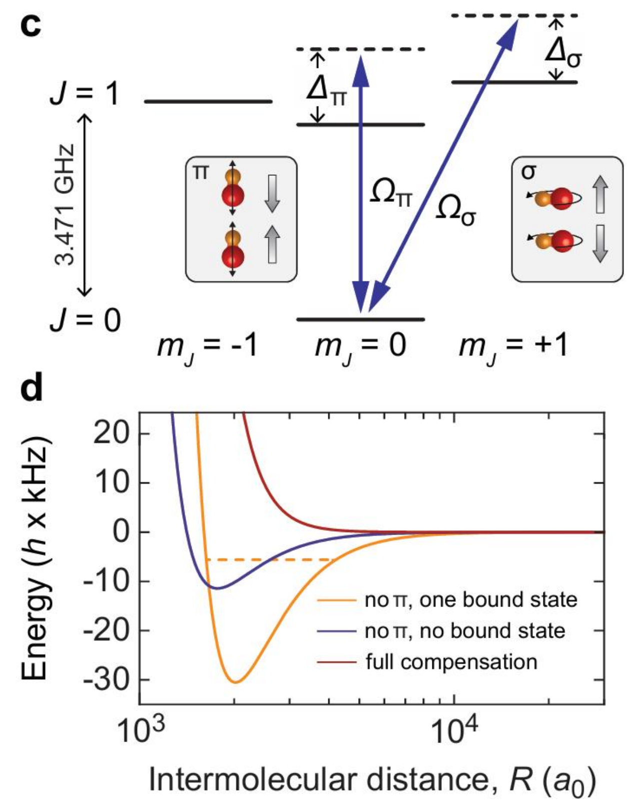
F. Deng *et al.*, arXiv:2405.13645

# Bosonic MSPMs

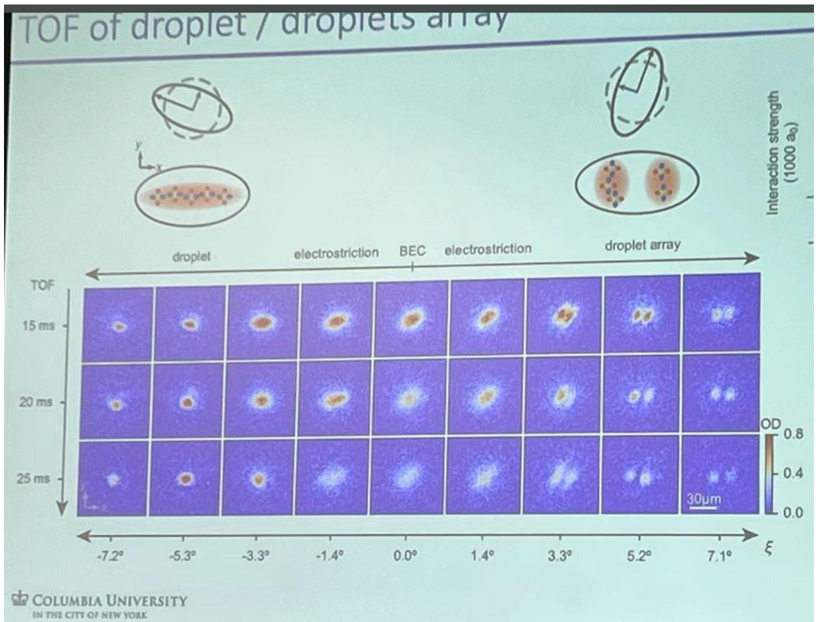
# Bose molecules

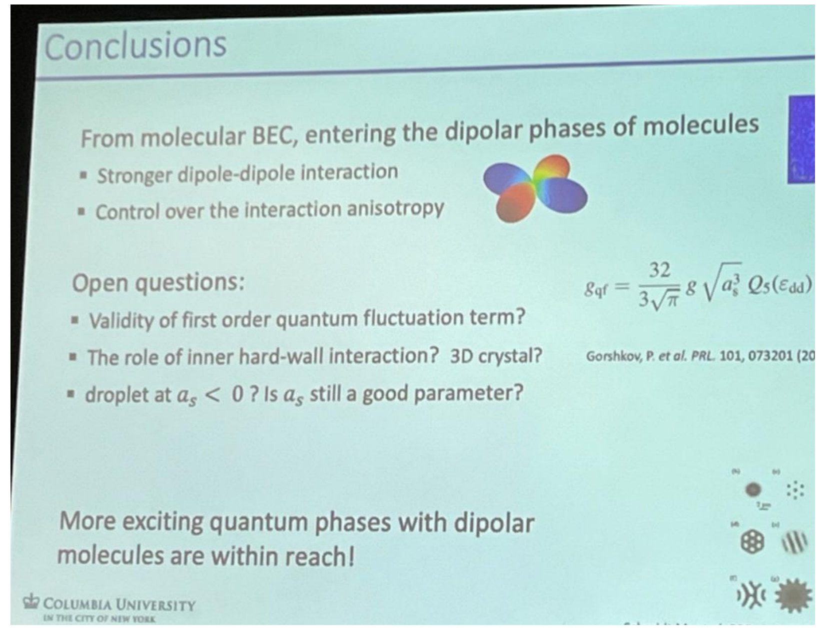



N. Bigagli *et al*., Nature 631, 289 (2024).



# Bose molecules




***DAMOP S. Will's talk***

# Bose molecules

***Hamiltonian:***

W. Jin *et al.*, arXiv:2406.06412

$$H = H_0 + H_{\text{int}},$$

$$H_0 = \int d\mathbf{r} \left[ \frac{1}{2M} \nabla \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r}) + V(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right]$$

$$H_{\text{int}} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}),$$

$$U(\mathbf{r}) = \frac{C_3}{r^3}(3\cos^2\theta - 1) + \frac{C_6}{r^6} \sin^2\theta (1 + \cos^2\theta),$$

$$U_{\text{pp}}(\mathbf{r}) = \frac{4\pi\hbar^2 a_s}{M} \delta(\mathbf{r}) + \frac{C_3}{r^3}(3\cos^2\theta - 1).$$

# Bose molecules

***Hamiltonian:***

W. Jin *et al.*, arXiv:2406.06412

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$$H_0 = \int d\mathbf{r} \left[ \frac{1}{2M} \nabla \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r}) + V(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right]$$

$$H_{\rm int} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}),$$

$$U(\mathbf{r}) = \frac{C_3}{r^3}(3\cos^2\theta - 1) + \frac{C_6}{r^6}\sin^2\theta(1+\cos^2\theta),$$

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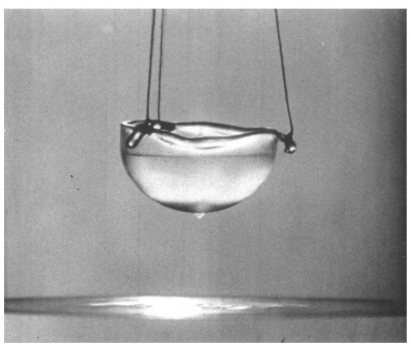
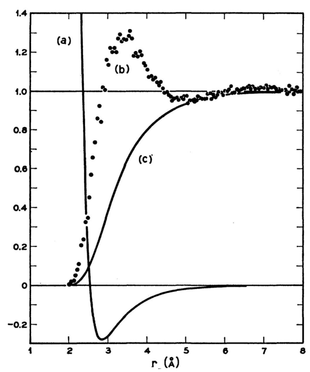
***Inapplicable!!!***



Liquid Helium




W. L. McMillan,
Phys. Rev. **138** A442 (1965)

$$g_2(\mathbf{r}, \mathbf{r}') = \frac{\langle \Psi | \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) | \Psi \rangle}{n(\mathbf{r}) n(\mathbf{r}')},$$

# Bose molecules

W. Jin *et al.*, arXiv:2406.06412

$$U(\mathbf{r}) = \frac{C_3}{r^3}(3\cos^2\theta - 1) + \frac{C_6}{r^6}\sin^2\theta(1+\cos^2\theta),$$

***Variational ansatz:***

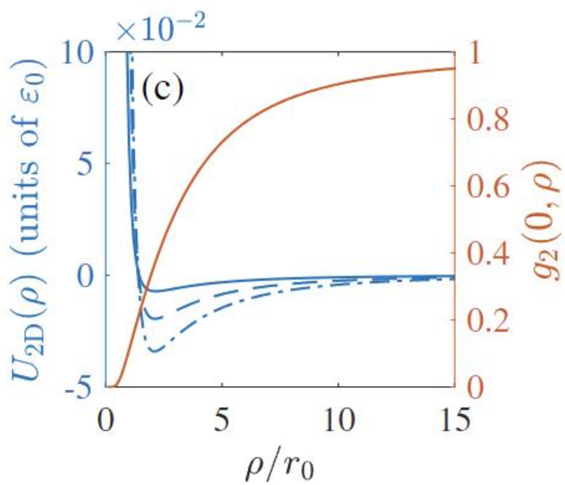
$$|\Psi\rangle = e^{-\alpha^2/2} e^{\alpha \hat{b}^\dagger} |0\rangle$$

$$\hat{b} = \int d\mathbf{r} \phi_0(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

$$|\Psi\rangle = S\,|\alpha\rangle / \sqrt{\mathcal{N}}$$

$$S = \exp[\frac{1}{2}\int d\mathbf{r} d\mathbf{r}' \chi(\mathbf{r},\mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})]$$

*TS, E. Demler, and J. I. Cirac, Annals of Physics **390**, 245 (2018).*
*TS, E. Demler, and J. I. Cirac, PRL **125**, 180602 (2020).*




$$|\Psi_N\rangle = \frac{1}{\sqrt{\mathcal{N}}} \int D[\mathbf{r}] \prod_{i<j(=1)}^{N} J(\mathbf{r}_i, \mathbf{r}_j) \prod_{j=1}^{N} \phi_0(\mathbf{r}_j) \hat{\psi}^\dagger(\mathbf{r}_j) |0\rangle$$

R. Jastrow, Phys. Rev. **98**, 1479 (1955).

# Bose molecules

***Ground state energy:***

$$E = \frac{1}{2M}\int d\mathbf{r}\nabla\phi(\mathbf{r})\nabla\phi(\mathbf{r}) - \int d\mathbf{r}d\mathbf{r}'\frac{1}{4M}\nabla\ln J(\mathbf{r},\mathbf{r}')\nabla\ln n(\mathbf{r})G_2(\mathbf{r},\mathbf{r}')$$
$$-\int d\mathbf{r}d\mathbf{r}'\frac{1}{4M}\nabla^2\ln J(\mathbf{r},\mathbf{r}')G_2(\mathbf{r},\mathbf{r}') + \int d\mathbf{x}V(\mathbf{r})n(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')G_2(\mathbf{r},\mathbf{r}'),$$

***Cluster expansions:***

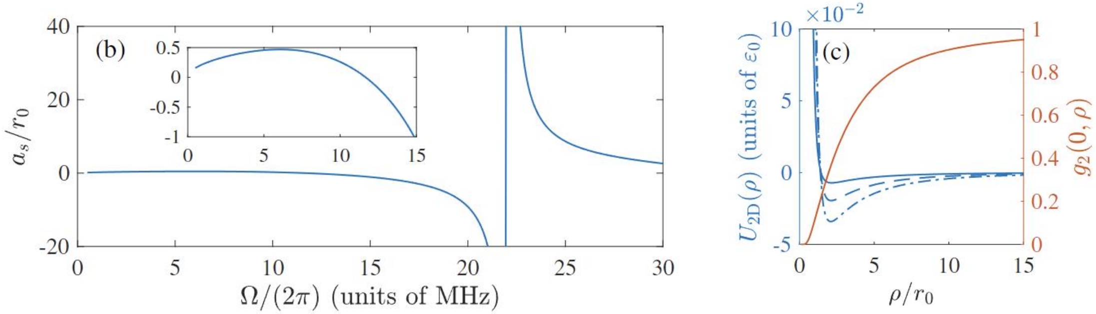
*J. B. Aviles, Annals of Physics 5, 251 (1958)*

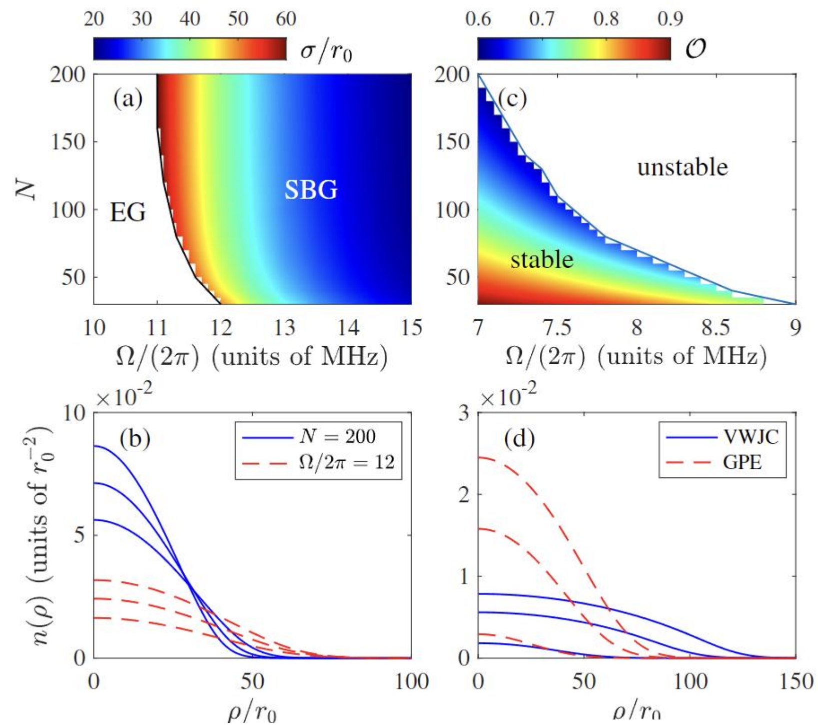
$$G_2(\mathbf{r},\mathbf{r}') = n(\mathbf{r})n(\mathbf{r}')J^2(\mathbf{r},\mathbf{r}')[1 + \int d\mathbf{r}_1 f(\mathbf{r},\mathbf{r}_1)n(\mathbf{r}_1)F(\mathbf{r}_1,\mathbf{r}')].$$

$$f(\mathbf{r}_i,\mathbf{r}_j) = J^2(\mathbf{r}_i,\mathbf{r}_j) - 1$$

# Bose molecules

***Phase diagrams:***



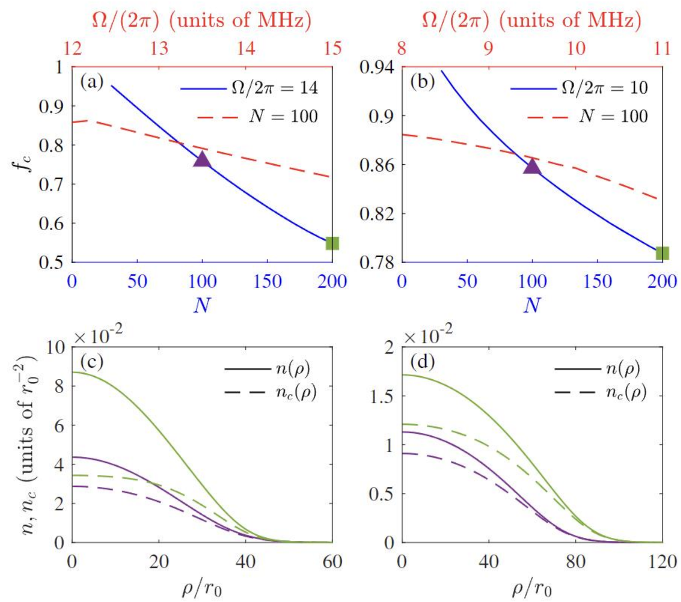



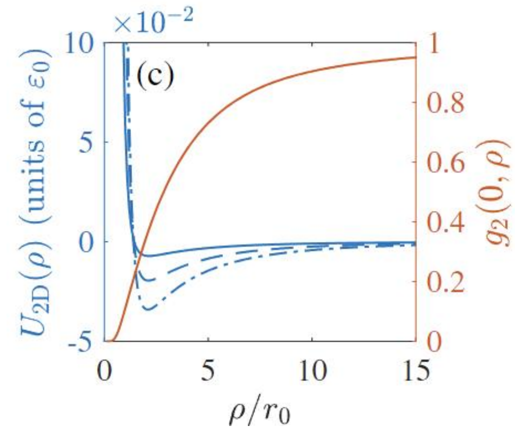

$$U(\mathbf{r}) = \frac{C_3}{r^3}(3\cos^2\theta - 1) + \frac{C_6}{r^6}\sin^2\theta(1+\cos^2\theta), \qquad U_{\rm pp}(\mathbf{r}) = \frac{4\pi\hbar^2 a_s}{M}\delta(\mathbf{r}) + \frac{C_3}{r^3}(3\cos^2\theta - 1).$$

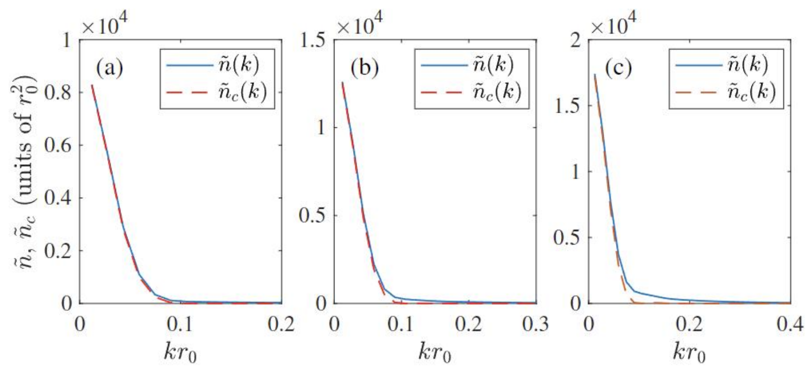
# Bose molecules

## *Condensate fractions and momentum distributions*

$$G_1(\boldsymbol{\rho},\boldsymbol{\rho}') = \langle\Psi|\hat{\psi}^\dagger(\boldsymbol{\rho}')\hat{\psi}(\boldsymbol{\rho})|\Psi\rangle = \sum_{\ell\geq 0} N_\ell\bar{\varphi}_\ell(\boldsymbol{\rho})\bar{\varphi}^*_\ell(\boldsymbol{\rho}')$$

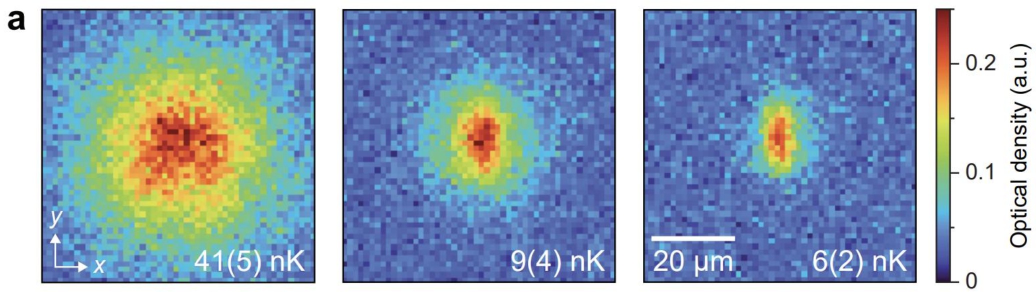


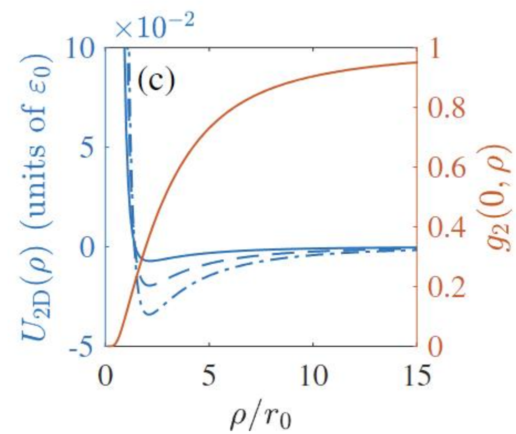



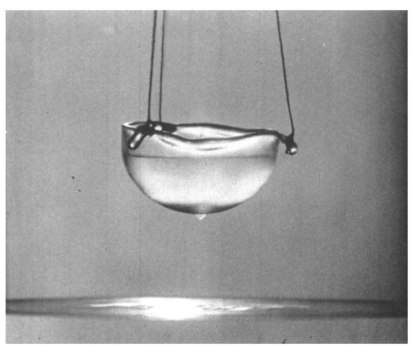
# Bose molecules

## ***Helium 4 v.s. MSPMs***

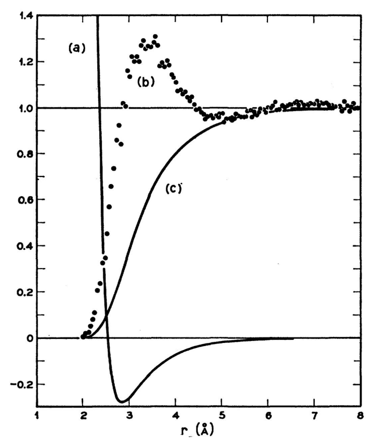



N. Bigagli *et al*., Nature 631, 289 (2024).



Liquid Helium




W. L. McMillan,
Phys. Rev. **138** A442 (1965)

# Conclusion and Outlook

New paradigm in MS polar molecules beyond atoms and Helium

F. Deng, et al., PRL 130, 183001 (2023)

J. Lin et al., Phys. Rev. X **13**, 031032 (2023)

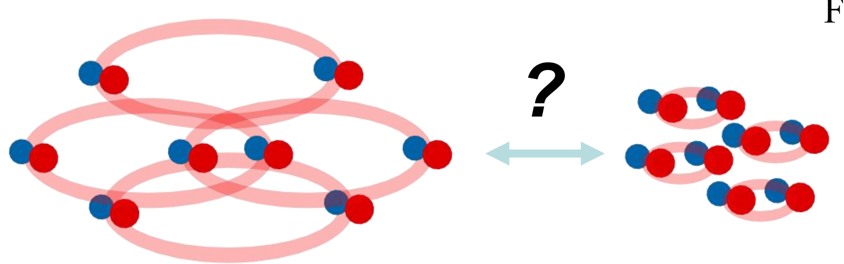
N. Bigagli *et al.*, Nature 631, 289 (2024).

W. Jin *et al.*, arXiv:2406.06412

T. Langen *et al.*,arXiv:2407.09391

Realization of tetramer BEC and BCS-BEC crossover

X. Y. Chen et al., Nature 626, 283 (2024)
F. Deng *et al.*, arXiv:2405.13645



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Dr. Xinyu Luo (MPQ)

Dr. Xingyan Chen (MPQ)

NaK group in MPQ


Thank you!