Quantum phases of bosonic chiral molecules in helicity lattices

Felipe Isaule
School of Physics and Astronomy
University of Glasgow

Collaborators:
R. Bennett and J. B. Götte
University of Glasgow

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felipeisaule.github.io felipe.isaulerodriguez@glasgow.ac.uk felipeisaule

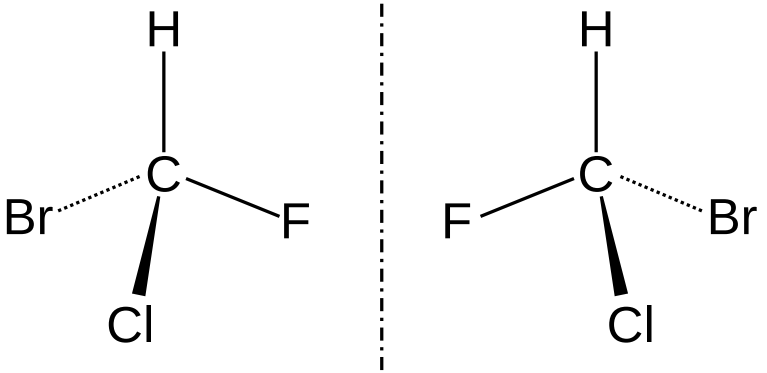
Outline

We present an exploratory study of the phase diagram of cold **chiral molecules** immersed in recently proposed **helicity lattices**.

1. Chiral molecules and helicity
2. Cold chiral molecules in optical helicity lattices
3. Conclusions and outlook

Chiral molecules

- Chiral molecules **cannot be superposed with their mirror image** by rotations and translations.
- Their left- and right-handed forms are referred to as **enantiomers**.



Bromochlorofluoromethane

- **Chiral discrimination**, the ability to separate enantiomers, has received significant interdisciplinary interest.
  D. Patterson and M. Schnell, Phys. Chem. Chem. Phys. **16**, 11114 (2014).
- In this direction, the use of **light**, which is by itself chiral, has received special attention to harness chiral molecules.

Optical helicity

- The **optical helicity** is defined as (in natural units)

$$\mathcal{H} = \frac{1}{2} \int d^3x \, (\boldsymbol{A} \cdot \boldsymbol{B} - \boldsymbol{C} \cdot \boldsymbol{E}) \ .$$

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}$$
$$\boldsymbol{E} = -\nabla \times \boldsymbol{C}$$

Classically, it measures the “twist” of the fields around the axis of propagation.

S. M. Barnett, R. P. Cameron, and A. M. Yao, PRA **86**, 013845 (2012).

- The integrand *h* is referred to as the **helicity density**

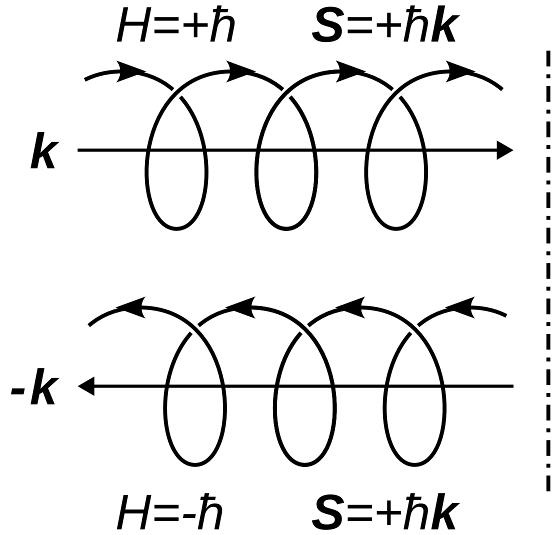
$$h = \frac{1}{2} (\boldsymbol{A} \cdot \boldsymbol{B} - \boldsymbol{C} \cdot \boldsymbol{E}) \ .$$

Optical helicity and spin

- The helicity is closely connected to the **spin of light**.
- The familiar definition of *H* as the projection of the spin in the direction of propagation can be seen from the quantised forms

$$\hat{\mathcal{H}} = \hbar \sum_{\boldsymbol{k}} \left(\hat{n}^{L}_{\boldsymbol{k}} - \hat{n}^{R}_{\boldsymbol{k}}\right) \ ,$$

$$\hat{\mathcal{S}} = \hbar \sum_{\boldsymbol{k}} \frac{\boldsymbol{k}}{|\boldsymbol{k}|} \left(\hat{n}^{L}_{\boldsymbol{k}} - \hat{n}^{R}_{\boldsymbol{k}}\right) \ .$$



S. M. Barnett, R. P. Cameron, and A. M. Yao, PRA **86**, 013845 (2012).

Discriminatory force

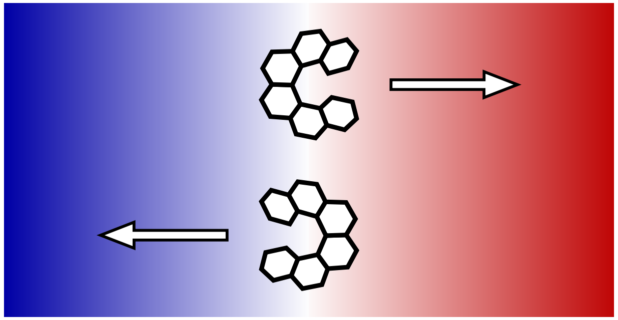
- The gradient of the helicity density exerts a **discriminatory force** on chiral molecules. To leading order, this force reads

$$\boldsymbol{F} = b_\chi \nabla h \,.$$

R. P. Cameron, S. M. Barnett, and A. M. Yao, NJP **16**, 013020 (2014).

- The constant *b* depends on molecular properties and has the **opposite sign** to that of the opposite enantiomer

$$b_L = -b_R \,.$$



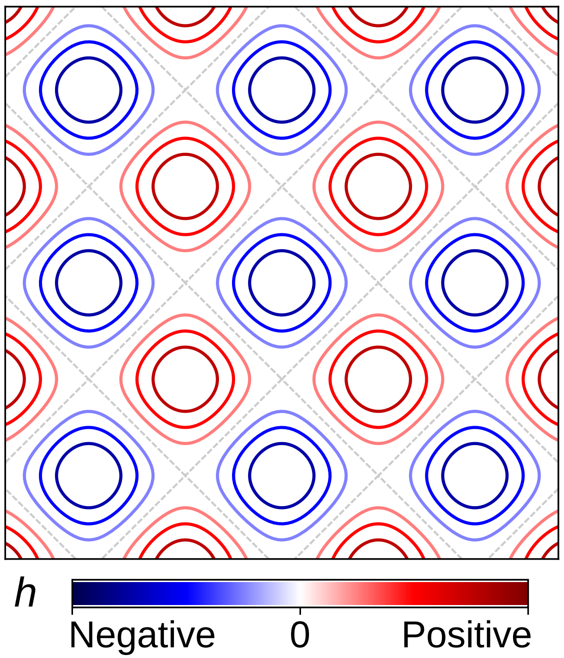
- Engineered light with varying helicity is a proposed mechanism for separating chiral molecules.

Helicity lattices

- **Superpositions** of coherent light waves can be used to create patterns with an oscillatory helicity density.
  K. C. van Kruining, R. P. Cameron, and J. B. Götte, Optica **5**, 1091 (2018).

- However, they have a homogeneous mean square of the electric field.

- We call them **helicity lattices**.



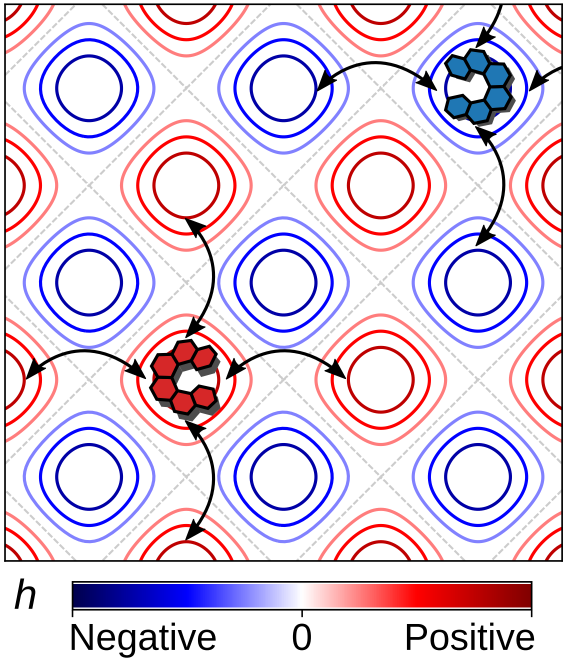
- **Cold chiral molecules** immersed in helicity lattices should show phases induced by their chirality.

- Trapping of chiral molecules at ultracold temperatures has not yet been achieved, but there is rapid progress realising cold polyatomic molecules.
  L. Anderegg *et al.*, Nat. Phys. **14**, 890 (2018).
  J. Kłos and S. Kotochigova, PRR **2**, 013384 (2020).
  B. L. Augenbraun, J. M. Doyle, T. Zelevinsky, and I. Kozyryev, PRX **10**, 031022 (2020).

Outline

1. Chiral molecules and helicity
2. **Cold chiral molecules in optical helicity lattices**
3. Conclusions and outlook

Cold chiral molecules in helicity lattices



- The chirality of a molecule determines if it is **attracted or repelled** from a given site.
  A. Canaguier-Durand *et al.*, NJP **15**, 123037 (2013).

- The molecules are immersed in a **periodic potential** with wells at the sites with **favourable helicity**.

- Potential depth:

$$V_0 \approx \frac{|G'|I}{\epsilon_0 c^2}\,.$$

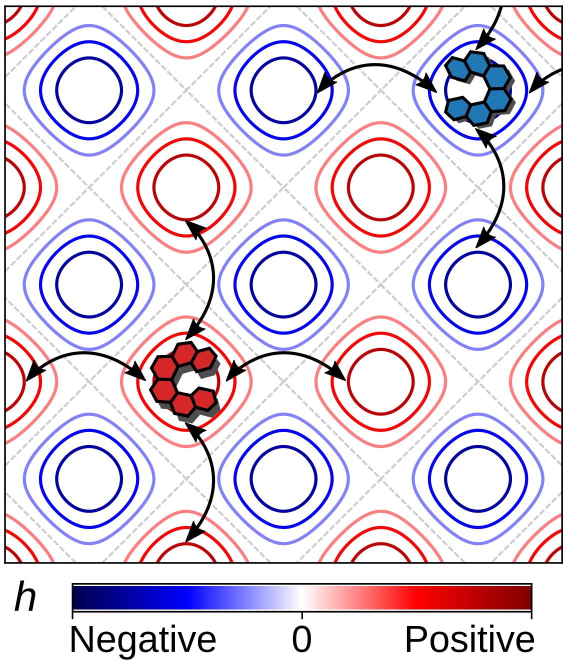
G' : electric dipole–magnetic Dipole optical activity tensor
I : Laser's intensity

R. P. Cameron *et al.*, Philos. Trans. R. Soc., A **375**, 20150433 (2017).

- By using $I \approx 10^9$ W/cm^2, a lattice with a spacing $\lambda \approx \mu$m in the μK regime forms a **tight lattice** which can be modelled with a **Hubbard-like model**.

- We study molecules immersed in a square 2D helicity lattice.

Model



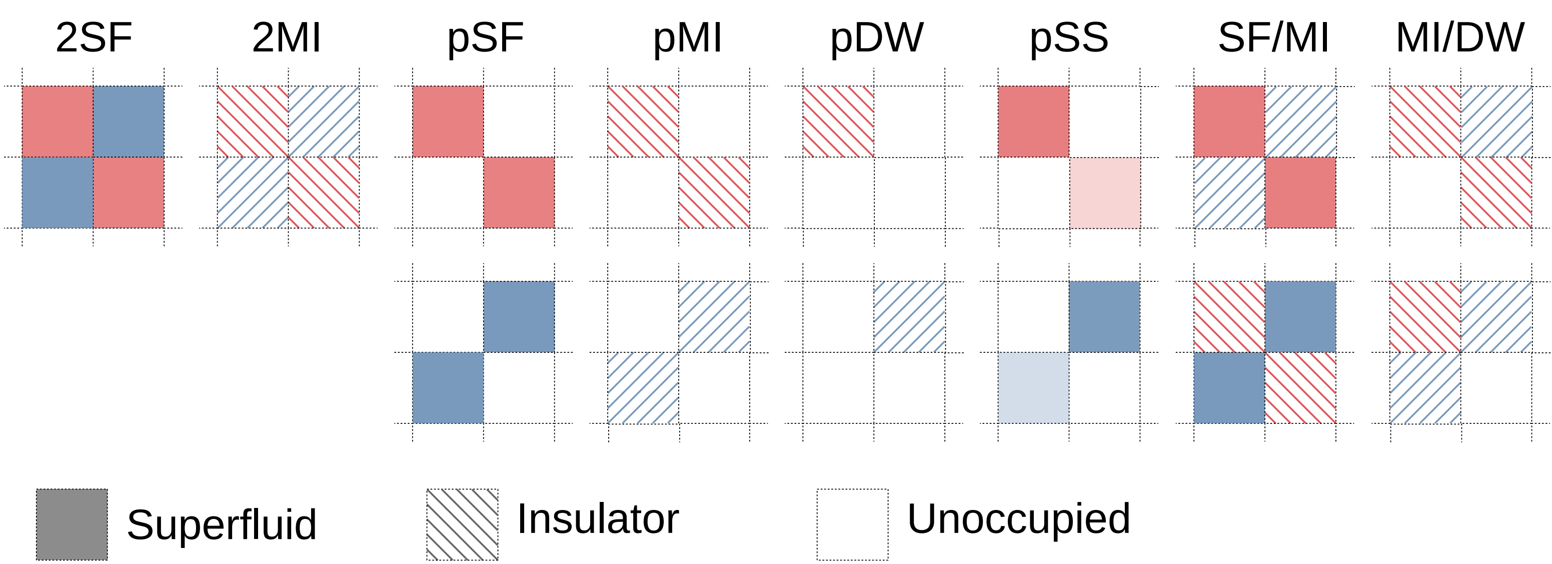
- We model the molecules as **point bosonic particles** (ground rovibrational state).
- The molecules interact through **dipole-dipole interactions**.
  D. P. Craig and T. Thirunamachandran, Theor. Chim. Acta **102**, 112 (1999).
- We consider dipoles polarised orthogonal to the lattice plane (**repulsive interactions**).

$$\hat{H} = -\frac{t}{2} \sum_{\langle\langle i,j \rangle\rangle_\chi} \left(\hat{b}^*_{\chi,i} \hat{b}_{\chi,j} + \hat{b}^*_{\chi,i} \hat{b}_{\chi,j} \right)$$
$$+ \frac{U}{2} \sum_i \hat{n}_{\chi,i} (\hat{n}_{\chi,i} - 1) + \frac{V_{LR}}{2} \sum_{\langle i,j \rangle_{LR}} \hat{n}_{\chi,i} \hat{n}_{\chi',j} + \frac{V}{2^{5/2}} \sum_{\langle\langle i,j \rangle\rangle_\chi} \hat{n}_{\chi,i} \hat{n}_{\chi,j}$$

- We study the phase diagram with a **Gutzwiller ansatz**.
  D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, PRL **81**, 3108 (1998).

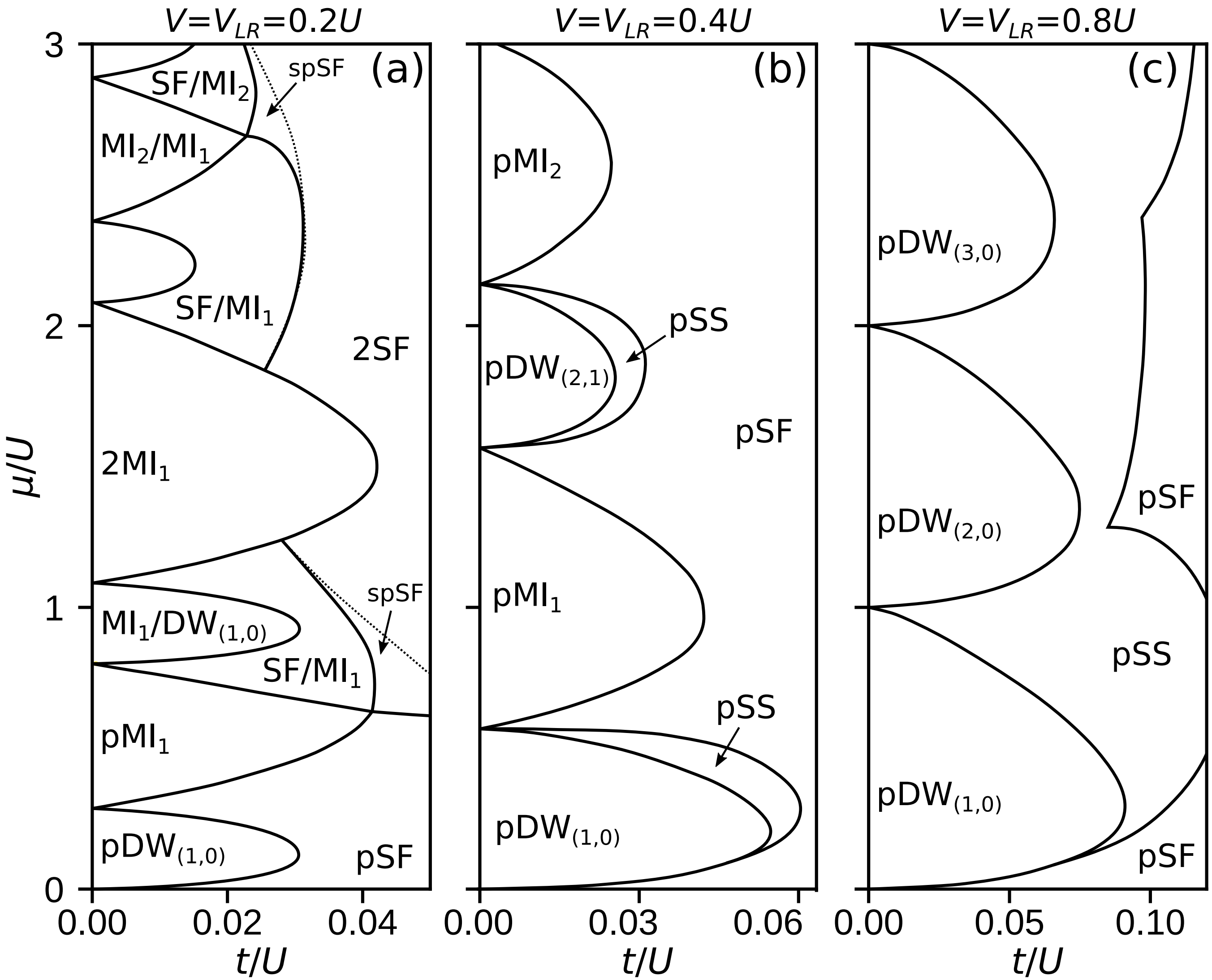
Quantum phases

- We identify the phases by examining the order parameter ϕ_i and occupancy n_i per site.
- Dipole-dipole interactions induce checker-board phases with **staggered occupation**.



SF: Superfluid
MI: Mott-insulator
DW: Density-wave
SS: Supersolid
p: polarised

Phase diagram



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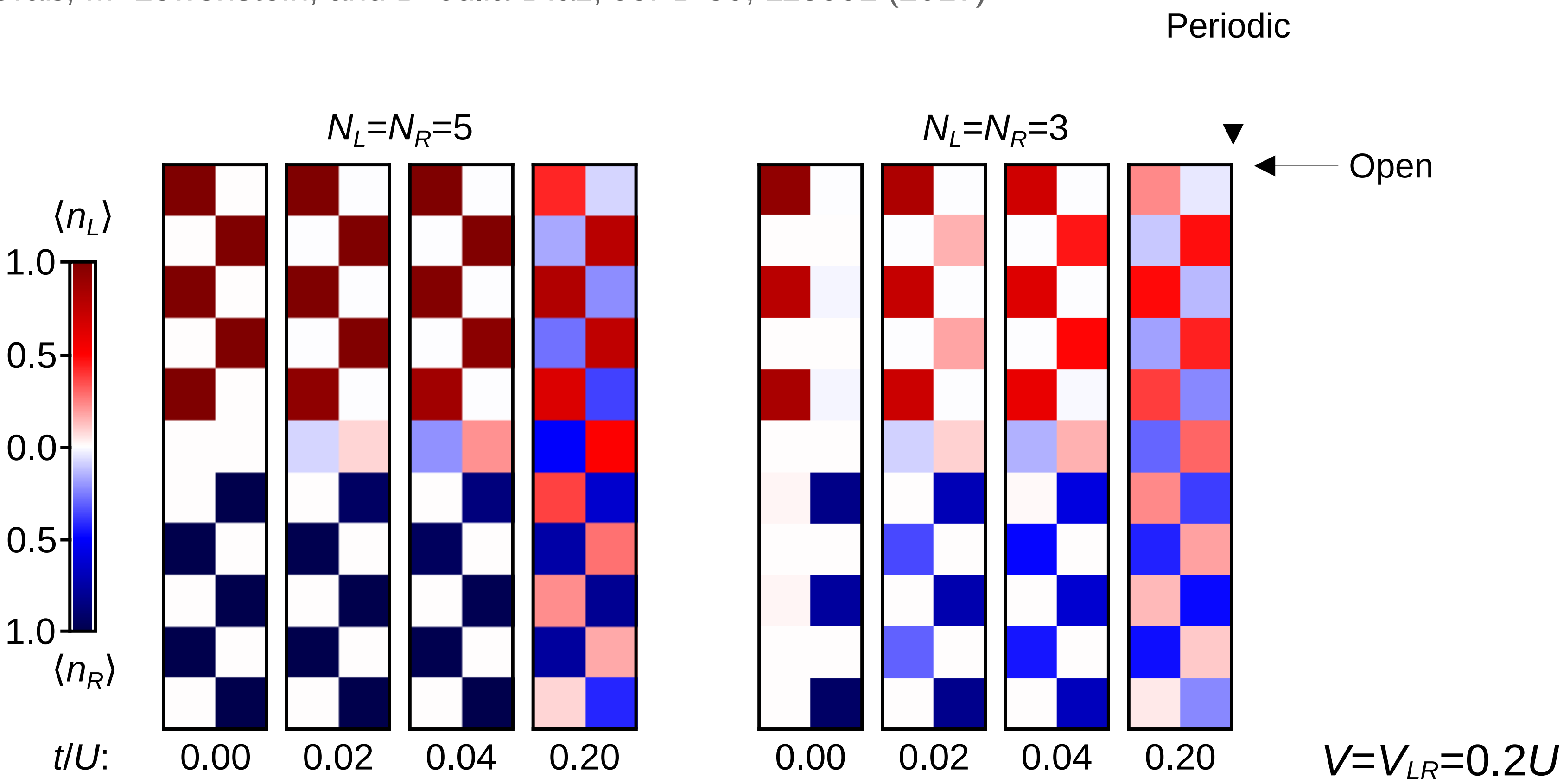
Phase separation

- In an experiment with a fixed density of molecules, the polarised phases produce a **phase separation** of enantiomers.

- We perform **exact diagonalisation** calculations for small lattices to illustrate this separation.

D. Raventós, T. Graß, M. Lewenstein, and B. Juliá-Díaz, JoPB **50**, 113001 (2017).



Conclusions

- Repulsive dipole-dipole interactions induce a rich phase diagram.
- In particular, a strong dipole-dipole repulsion induces a **left/right polarisation**, which opens a potential new avenue for **chiral discrimination**.
- <u>Future work:</u>
  - Consideration of realistic molecular interactions and internal structure (**molecular rotation**).
  - Employ **beyond mean-field** approaches and consideration of other geometries.

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More details: F. Isaule, R. Bennett, and J. B. Götte PRA **106**, 013321 (2022).
K. C. van Kruining, R. P. Cameron, and J. B. Götte, Optica **5**, 1091 (2018).