Quantum phases of bosonic chiral molecules in helicity lattices

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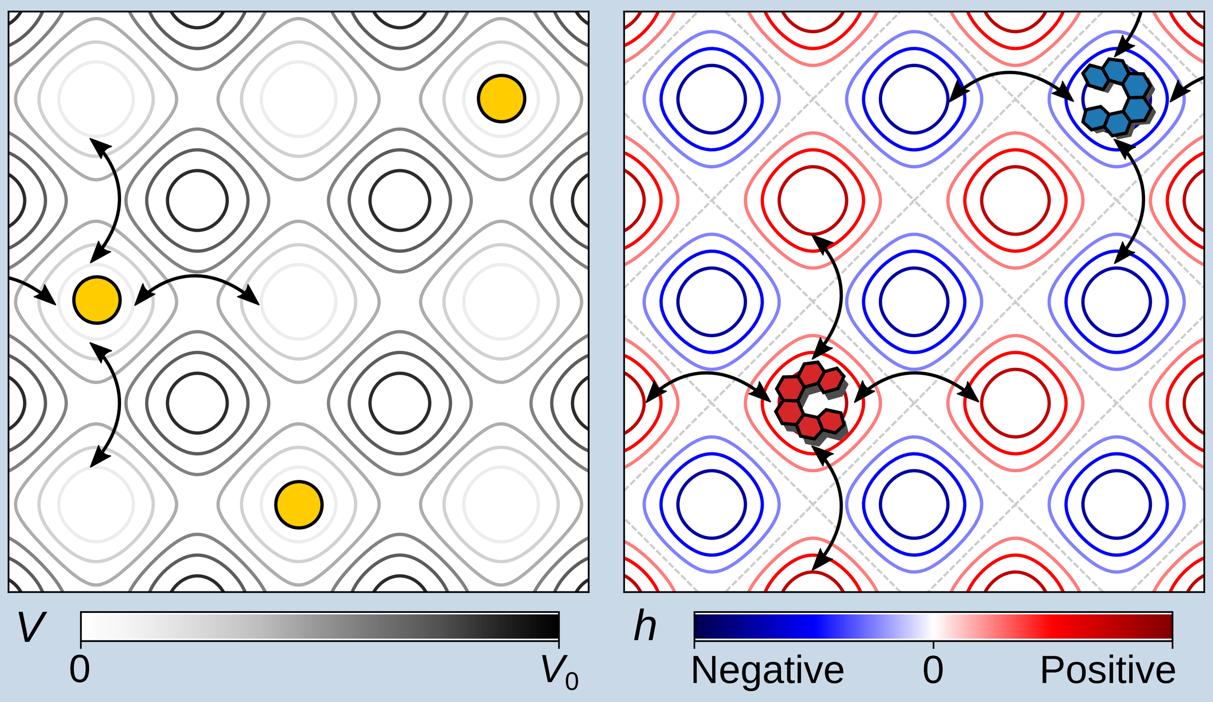
We reveal the existence of **polarizing phases** for the enantiomers of cold, interacting **chiral molecules** in a **helicity lattice.** These recently proposed lattices have **sites with alternating helicity** which exert a **discriminatory force** on chiral molecules. We find that a **strong dipolar repulsion** between molecules results in the **separation of left and right enantiomers**.

Background

Helicity lattices [1] are a new type of optical lattice which have perfectly homogeneous mean squared values of the electric field, but spatially **varying helicity** *h*. This helicity exerts a **discriminatory force** on chiral molecules with different handedness [2]. Therefore, the handedness of an enantiomer determines if it is **attracted or repelled from a given site**.



(Left): Illustration of a conventional optical lattice. Oscillating electric fields induce a periodic potential for atoms. (Right): Illustration of a square helicity lattice. Red and blue regions correspond to sites with opposite helicity densities *h* which induce a discriminatory force on enantiomers.

The recent progress in laser cooling has opened the possibility of **cooling and trapping polyatomic molecules** in the ultracold regime [3]. In particular, roadmaps for cooling chiral molecules have already been proposed [4,5]. This means that systems of ultracold chiral molecules in helicity lattices could be achieved in the near future, enabling the study of novel forms of chiral matter.

In this work, **we study systems of ultracold interacting chiral molecules immersed in square helicity lattices**. We tune parameters such as the dipole-dipole interaction strength and tunneling rates to study the **phase diagram** at low temperatures.

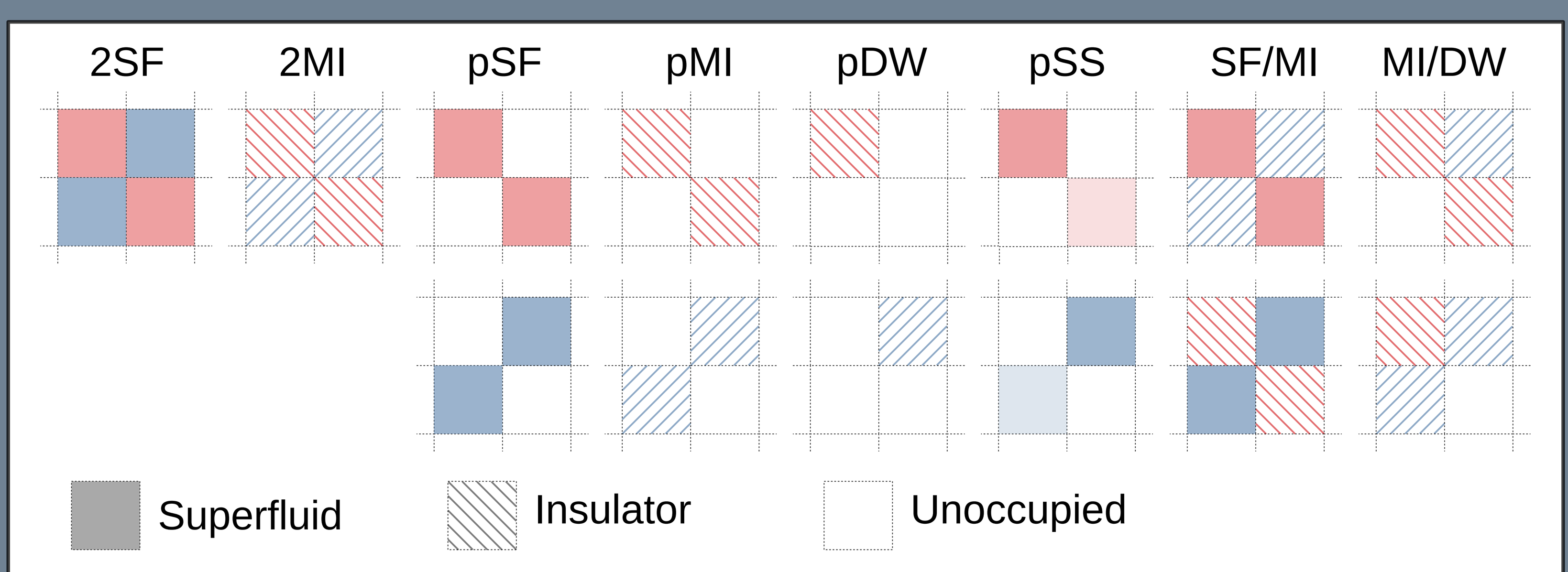
Model and quantum phases

We consider that the chiral molecules are point bosonic particles in their **ground robrivational state**. By assuming that the dipoles are polarized orthogonal to the lattice plane, we describe a tight helicity lattice with an **extended Bose-Hubbard model** [6]

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

where left/right (χ=L,R) **enantiomers can only tunnel to sites with favorable helicity**. In addition, we consider up to **next-to-nearest neighbor repulsive dipole-dipole interactions**.

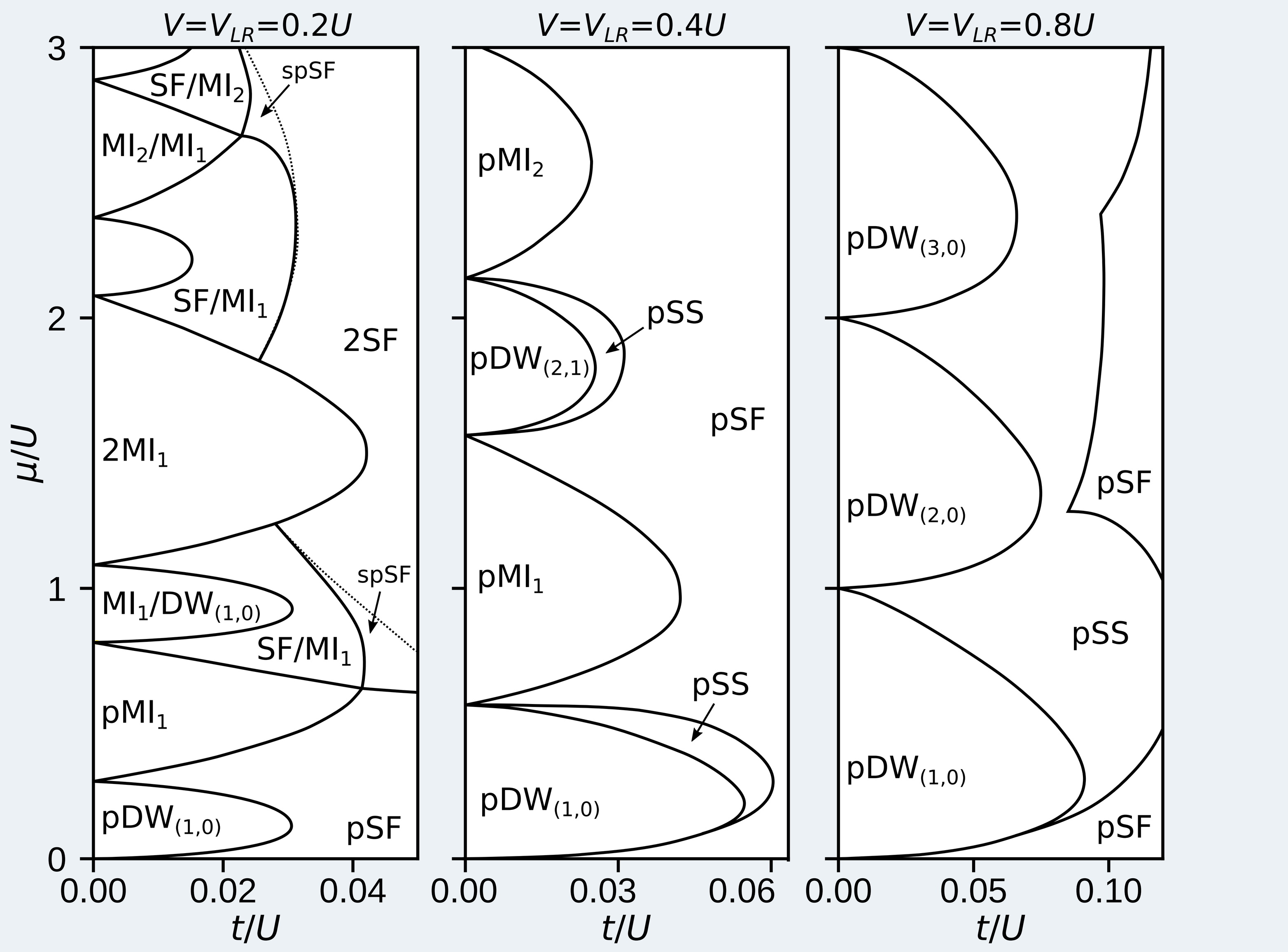
We study the phase diagram with the **Gutzwiller ansatz** [7]. We identify the phases by examing the order parameter ϕ_i and occupancy n_i per site. We illustrate some of these phases below.



Bosons show **superfluid** and **insulator** phases. In addition, dipole-dipole interactions induce checker-board phases with **staggered occupation** [7], producing a plethora of combinations.

Phase diagram

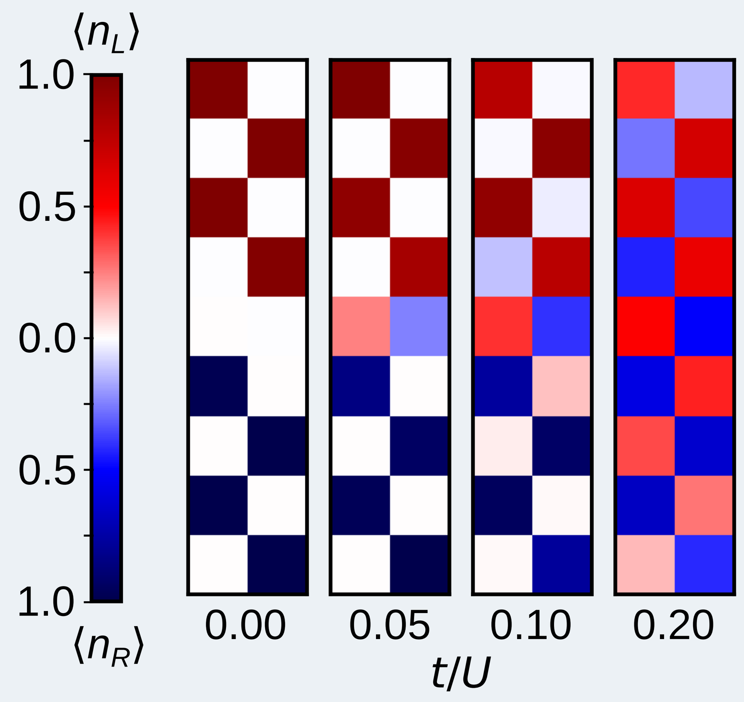
We find a rich phase diagram that depends strongly on V and V_{LR}. We show some representative diagrams below.



We find different combinations of insulator and superfluid phases. In particular, strong dipole-dipolar repulsion induces the **polarization of left/right molecules**.

In an experiment, such polarization would produce the **phase separation** of enantiomers, where each enantiomer species occupies different regions of the lattice. This separation can be seen as a method of **chiral discrimination** in the ultracold regime.

To illustrate this phase separation, we perform **exact diagonalization** of small lattices. We find that the lattice shows phase-separated superfluids and insulators for small *t* (see right figure), as expected.



Average occupation per site for $V=V_{LR}=0.2U$ obtained from exact diagonalization in a helicity lattice with 9x2 sites and four left and four right enantiomers. The x-axis is periodic, while the y-axis is finite.

Outlook

We have shown that repulsive dipolar interactions between chiral molecules immersed in helicity lattices can induce a plethora of quantum phases. In particular, we find phases with left/right polarization, as well as phases with asymmetric occupations.

Future work will include consideration of **realistic interactions** [9] between molecules, as well as effects from their internal structure such as from **molecular rotation** [10]. We will also employ beyond mean-field approaches to provide a better description.

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