Hard-core dipolar bosons in lattices with intermediate geometries between quadratic and triangular

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Hamiltonian

- hard-core extended Bose-Hubbard Hamiltonian

$$\hat{H} = -\sum_{i,j} J_{ij}\hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\sum_{i,j} V_{ij}\hat{n}_i\hat{n}_j - \mu\sum_i \hat{n}_i$$

describes hard-core dipolar bosons in a lattice.

- bosonic creation, annihilation and number operators for lattice site i: $\hat{a}_i^\dagger$, $\hat{a}_i$, $\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i$
- tunneling between lattice sites i and j: $J_{ij}\hat{a}_i^\dagger\hat{a}_j$
- interaction between lattice sites i and j: $\frac{1}{2}V_{ij}\hat{n}_i\hat{n}_j$
- chemical potential: μ
- hard-core: strong on-site repulsion $\Rightarrow$ not more than one particle per site

- For the lattices, that we investigate, the Hamiltonian can be rewritten:

$$\mathring{H} = -\mathring{J}\sum_{ij}\Gamma_{ij}\hat{a}_i^\dagger\hat{a}_j + \frac{1}{2}\sum_{ij}\Omega_{ij}\hat{n}_i\hat{n}_j - \mathring{\mu}\sum_i \hat{n}_i$$

according to

$$V := \sum_i V_{ij} = \sum_j V_{ij},\ J := \sum_i J_{ij} = \sum_j J_{ij}$$
$$\Omega_{ij} := \frac{V_{ij}}{V},\ \sum_i \Omega_{ij} = 1,\ \sum_j \Omega_{ij} = 1,\ \Gamma_{ij} := \frac{J_{ij}}{J},\ \sum_i \Gamma_{ij} = 1,\ \sum_j \Gamma_{ij} = 1$$
$$\mathring{H} = \frac{\hat{H}}{V},\ \mathring{J} = \frac{J}{V},\ \mathring{\mu} = \frac{\mu}{V}$$

- "$\circ$" stands for "unitless"
- creates useful scaling of phase diagram axes
- $\mathring{J}$, $\mathring{\mu}$: axes of phase diagram
- Γ_{ij}, Ω_{ij}: distribution of hopping and interaction respectively

Gutzwiller mean-field approximation

- product state approximation, normalization condition

$$|\psi\rangle = \bigotimes_i \left(c_{0i}|0_i\rangle + c_{1i}|1_i\rangle\right) \qquad |c_{0i}|^2 + |c_{1i}|^2 = 1 \quad \forall i$$

- expectation values (with respect to product state):

$$\langle\psi|\,\hat{n}_i\,|\psi\rangle = |c_{1i}|^2 =: \varrho_i \qquad \langle\psi|\,\hat{a}_i^\dagger\hat{a}_j\,|\psi\rangle = c_{0i}c_{1i}^*c_{0j}^*c_{1j} = \psi_i^*\psi_j$$
$$\langle\psi|\,\hat{a}_i\,|\psi\rangle = c_{0i}^*c_{1i} =: \psi_i \qquad \langle\psi|\,\hat{n}_i\hat{n}_j\,|\psi\rangle = |c_{1i}|^2\,|c_{1j}|^2 = \varrho_i\varrho_j$$

- energy expectation value (mean-field energy):

$$\mathring{E} = \langle\psi|\,\mathring{H}\,|\psi\rangle = -\mathring{J}\sum_{ij}\Gamma_{ij}\psi_i^*\psi_j + \frac{1}{2}\sum_{ij}\Omega_{ij}\varrho_i\varrho_j - \mathring{\mu}\sum_i \varrho_i$$

Numerical calculation

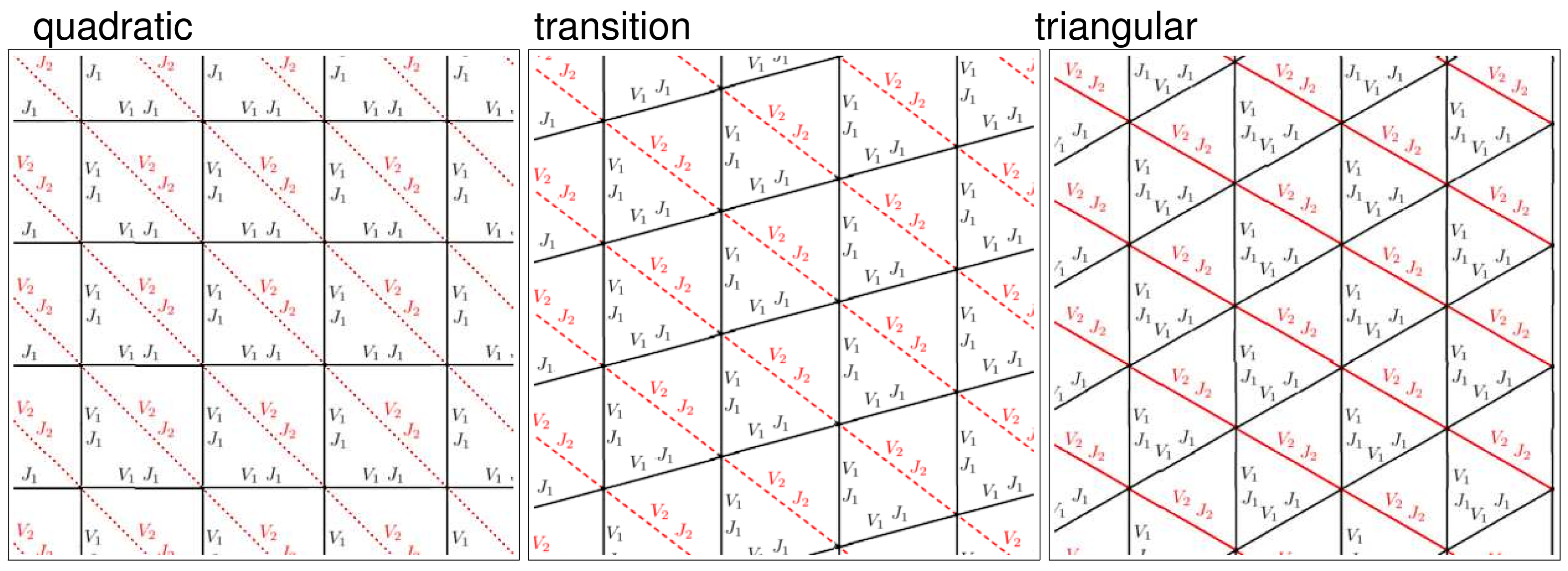
- substitution ensures, that normalization condition is fulfilled:

$$c_{0i} = \cos\alpha_i\, e^{i\varphi_{0i}} \qquad \varrho_i = |c_{1i}|^2 = \sin^2\alpha_i$$
$$c_{1i} = \sin\alpha_i\, e^{i\varphi_{1i}} \qquad \psi_i = c_{0i}^*c_{1i} = \cos\alpha_i\,\sin\alpha_i\, e^{i\varphi_i}$$
$$\varphi_i := \varphi_{0i} - \varphi_{1i}$$

- order parameters:
  - $\varrho_i \in \mathbb{R}$: density at lattice site i
  - $\psi_i \in \mathbb{C}$: indicator for superfluidity at lattice site i
- numerical calculation: minimalization of $\mathring{E}$ with respect to α_i's and φ_i's

Transition between quadratic and triangular lattice

quadratic | transition | triangular

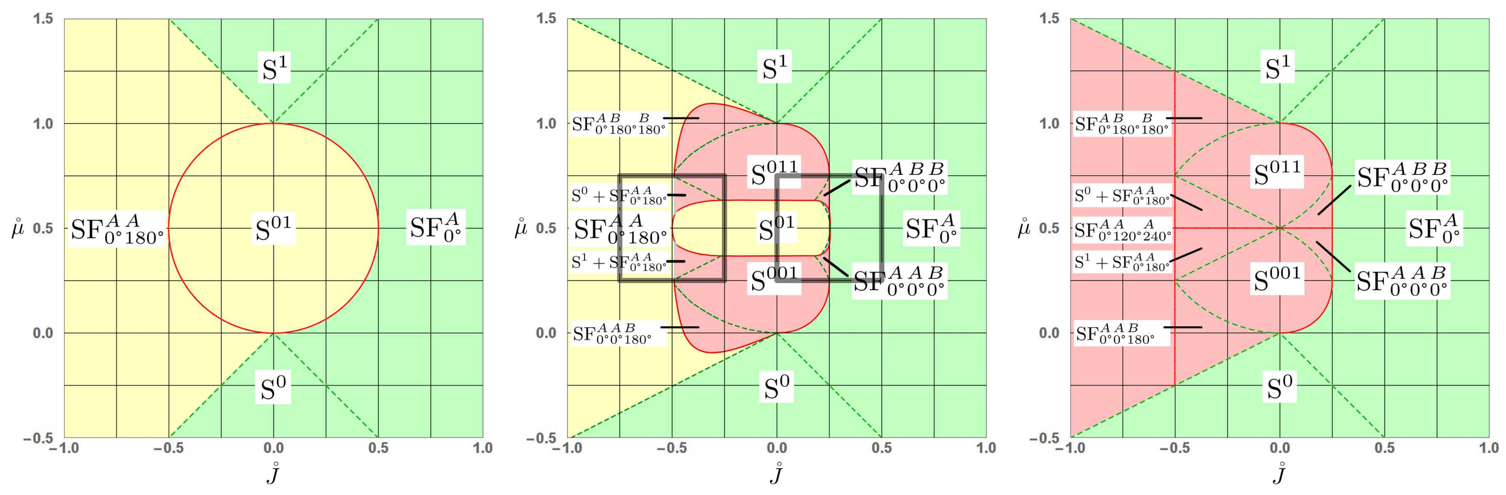


dotted:	dashed:	solid lines:
no interaction, no hopping	interaction and hopping smaller compared to solid lines	interaction and hopping to next-neighbors
$V_2 = 0$	$0 < V_2 < V_1$	$V_2 = V_1$
$J_2 = 0$	$0 < J_2 < J_1$	$J_2 = J_1$

- transition: interaction V_2 and hopping J_2 change relative to V_1 and J_1

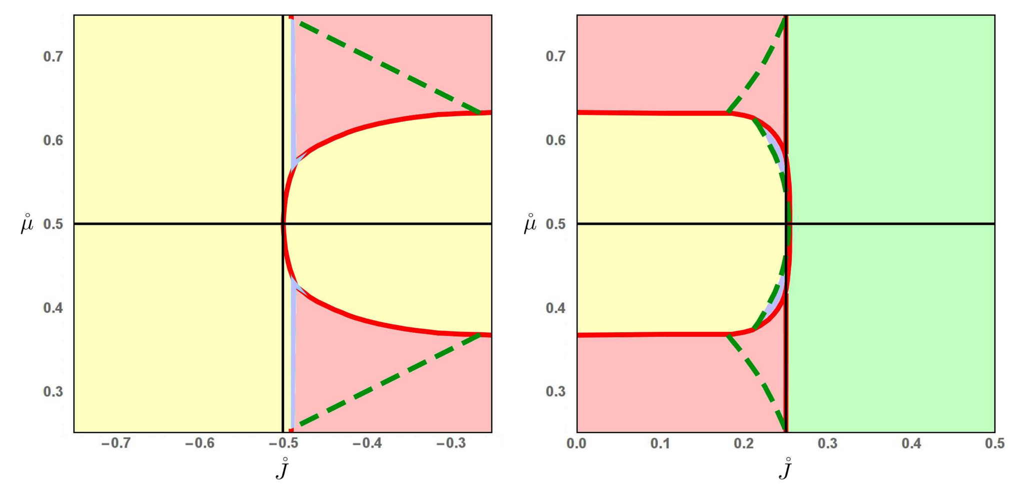
Whole phase diagram and 1st zoom

- green dashed lines: continuous phase transition
- red solid lines: discontinuous phase transition
- yellow areas: phases with spatial symmetry occurring in quadratic lattice
- red areas: phases with spatial symmetry occurring in triangular lattice
- green areas: phases with spatial symmetry occurring in both
- blue areas: phases with spatial symmetry occurring in neither (new phases)



quadratic	transition	triangular
$\frac{V_2}{V_1} = \frac{J_2}{J_1} = 0$	$\frac{V_2}{V_1} = \frac{J_2}{J_1} = 0.65$	$\frac{V_2}{V_1} = \frac{J_2}{J_1} = 1$

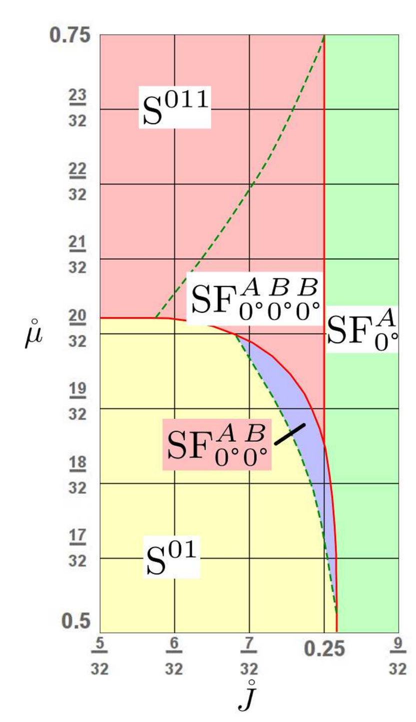
First zoom towards blue areas (see black rectangles in transition phase diagram):



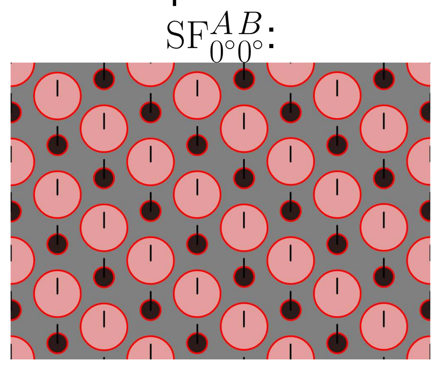
New phases for positive hopping and 2nd zoom

Visualization of spacial distributions (right image):

- HSV color space used for color-coding
- Size of circles and direction of lines used for geometric visualization
- Area of circles and brightness V: ϱ_i
- Length of lines and saturation S: $|\psi_i|$
- Direction of lines and hue H: $\arg\psi_i$ (complex phase of ψ_i)

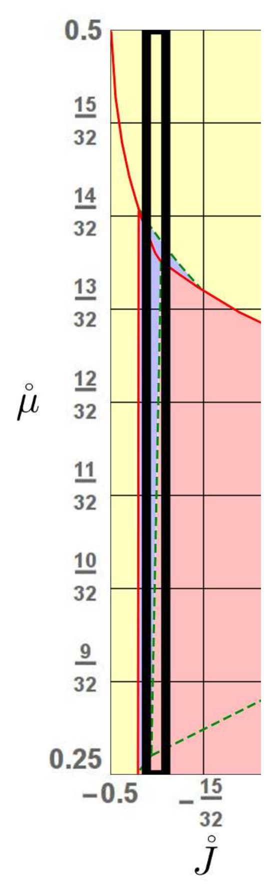


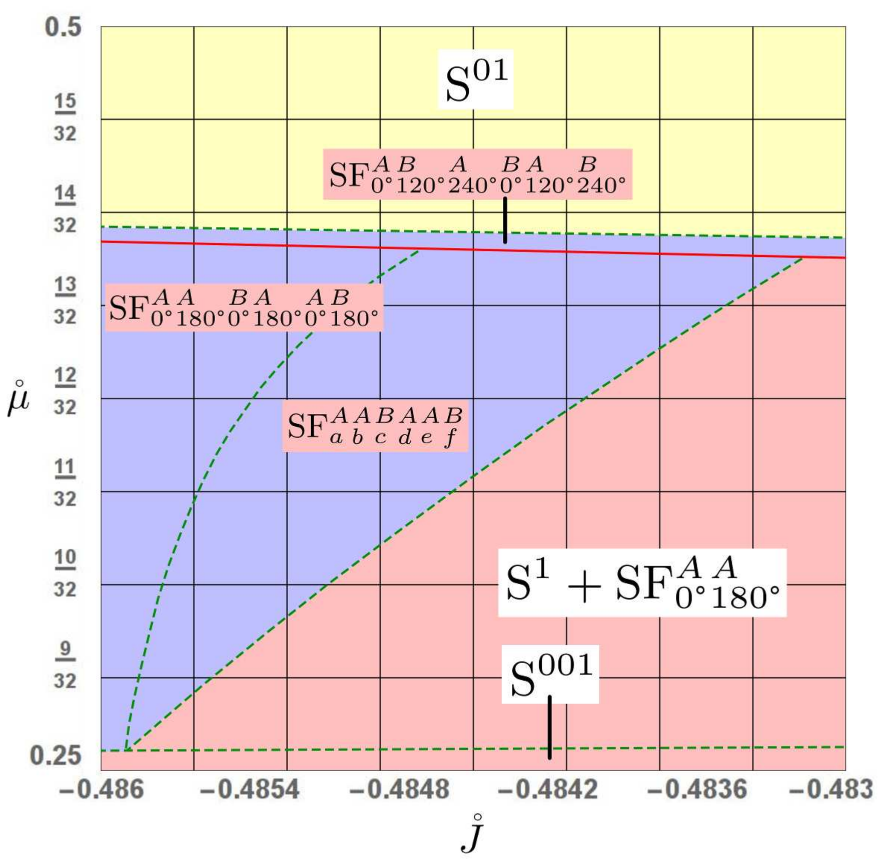
Supersolid:
$SF^{AB}_{0°0°}$:



- Stripe pattern
- all sites superfluid
- Pattern can be described with two sites in the unit cell

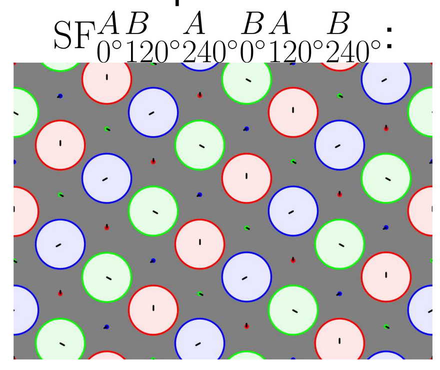
New phases for negative hopping, 2nd and 3rd zoom



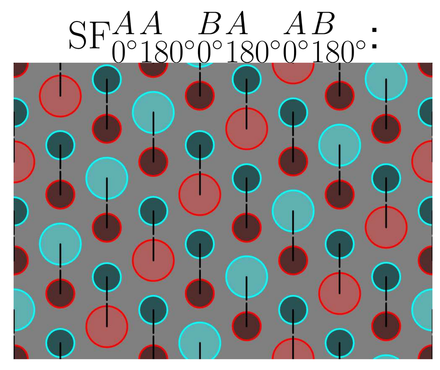


- Zoom into black rectangle from left image
- Scaled just in horizontal direction

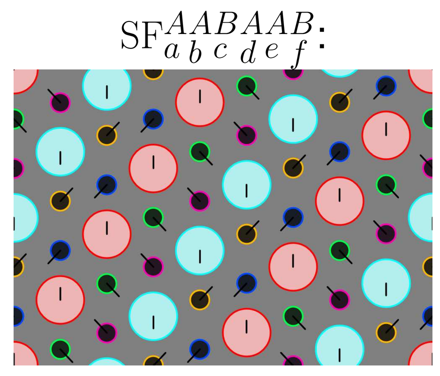
Supersolid:
$SF^{AB\ \ A\ \ BA\ \ B}_{0°120°240°0°120°240°}$:



$SF^{AA\ \ BA\ \ AB}_{0°180°0°180°0°180°}$:



$SF^{AABAAB}_{a\,b\,c\,d\,e\,f}$:



- Patterns can be described with six sites in the unit cell
- In the $SF^{AABAAB}_{a\,b\,c\,d\,e\,f}$ phase the complex phases of ψ_i are changing within the phase diagram, which doesn't happen for the quadratic or triangular lattice, but only here in the transition between both.