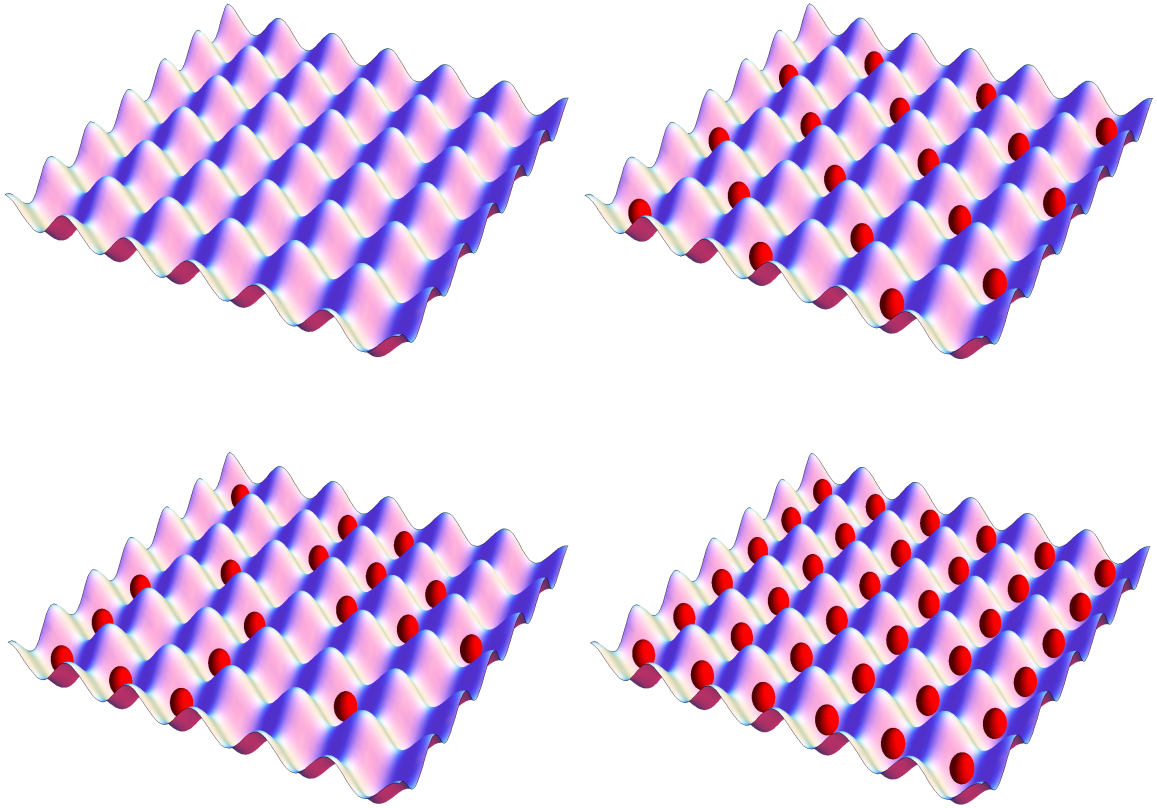
# Mean-field theory for extended Bose-Hubbard model with hard-core bosons



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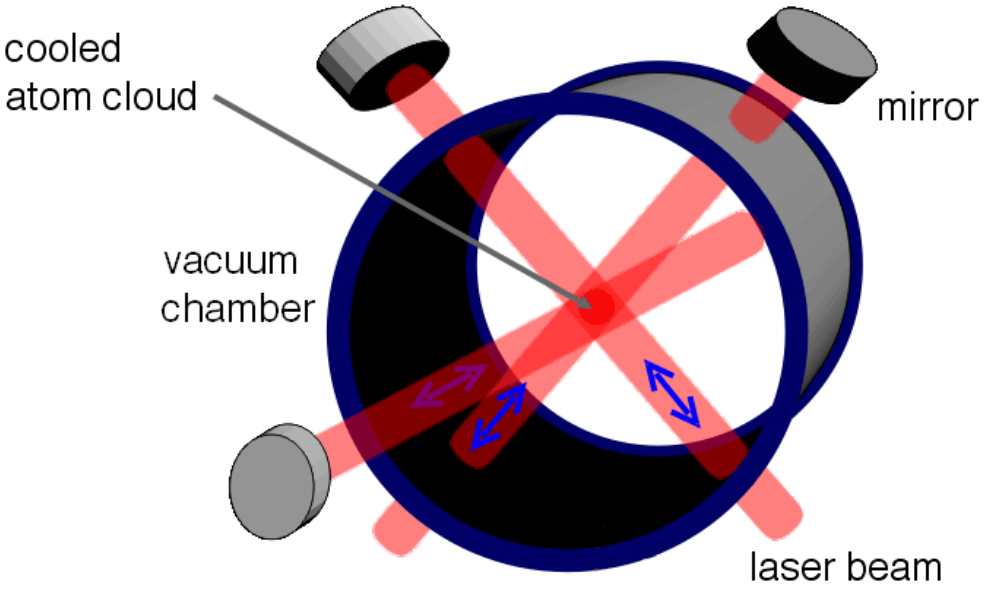
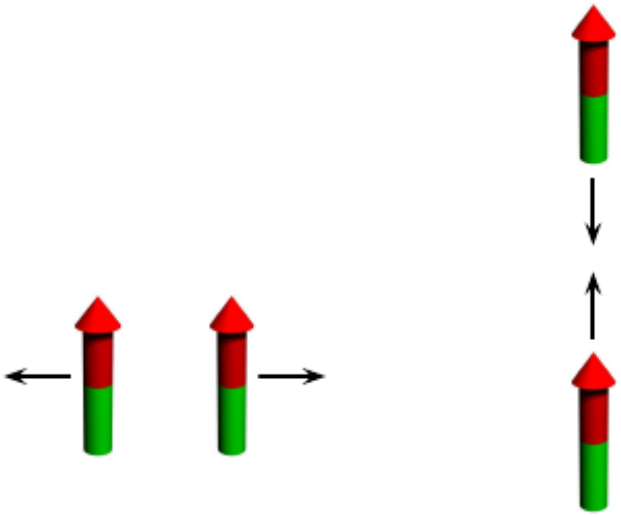
Technische Universität Kaiserslautern

# Outline

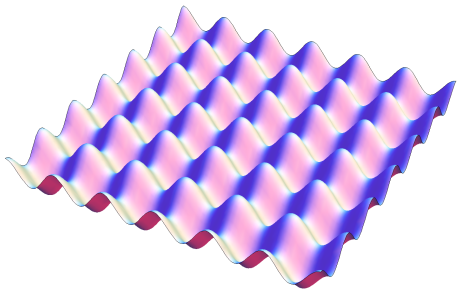
- Introduction
  - Experiment
  - Hamiltonian
  - Periodic patterns
- Main part
  - Mean-field (MF) **approximation** method
  - MF-**Hamiltonian** for unit cell in a periodic pattern (dependent on mean-field parameters)
  - **General calculation method** for any pattern
    - energy eigenvalues
    - mean-field parameters
  - **Results** (quadratic lattice, triangular lattice)
- Outlook
  - Completing mean-field for triangular lattice
  - Negative hopping $J$
  - Other lattices
  - Quantum corrections

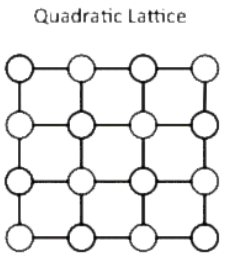
# Experiment

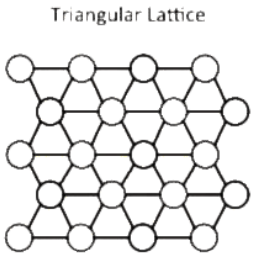


$$T \approx 0$$





# Hamiltonian

## Extended Bose-Hubbard model

$$\hat{H} = -J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1\right) - \mu \sum_i \hat{n}_i + \frac{V}{2} \sum_{<i,j>} \hat{n}_i \hat{n}_j$$

Hopping parameter $J$

$$J = J\left(i,j\right) = -\int d^3x \; w^* \left(\mathbf{x} - \mathbf{x_i}\right) \left[-\frac{\hbar^2}{2m} \triangle + V_{ext}\left(\mathbf{x}\right)\right] w\left(\mathbf{x} - \mathbf{x_j}\right)$$

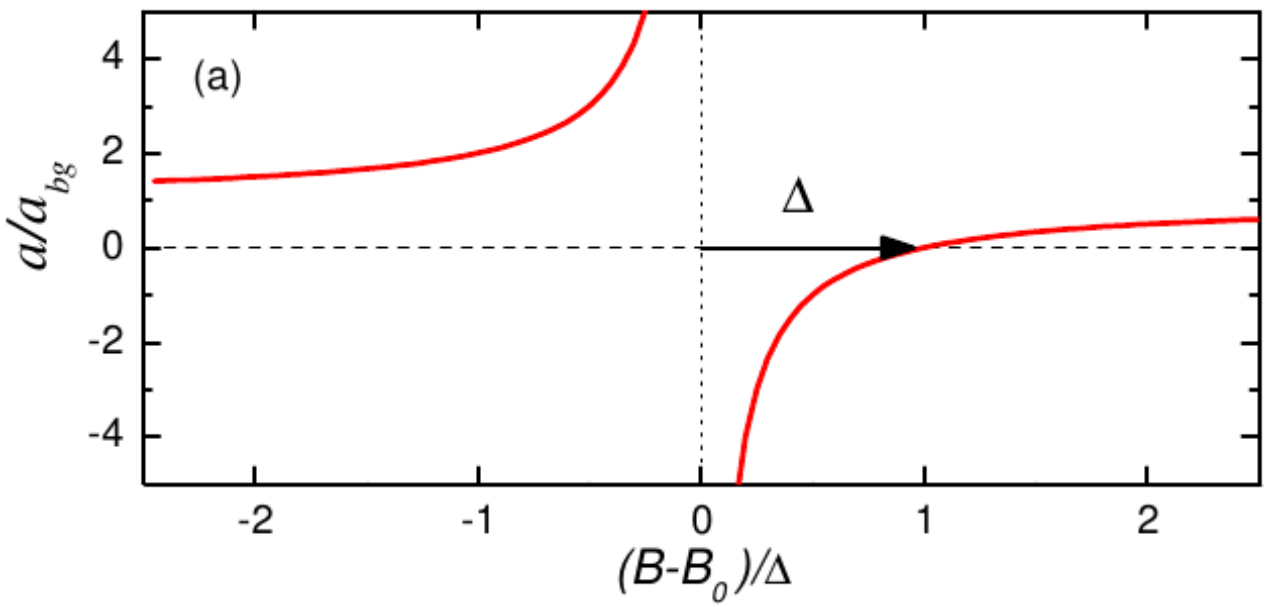
On-site interaction $U$

$$U = U\left(i\right) = \frac{4\pi a \hbar^2}{m} \int d^3x \; \left|w\left(\mathbf{x} - \mathbf{x_i}\right)\right|^4$$

Next neighbour interaction $V$

$$V = V\left(i,j\right) = \int d^3x \int d^3x' \; V_{dipol}\left(\mathbf{x}, \mathbf{x}'\right) \left|w\left(\mathbf{x} - \mathbf{x_i}\right)\right|^2 \left|w\left(\mathbf{x}' - \mathbf{x_j}\right)\right|^2$$

# Feshbach resonance




$$a(B) = a_{bg}\left(1 - \frac{\Delta}{B - B_0}\right)$$

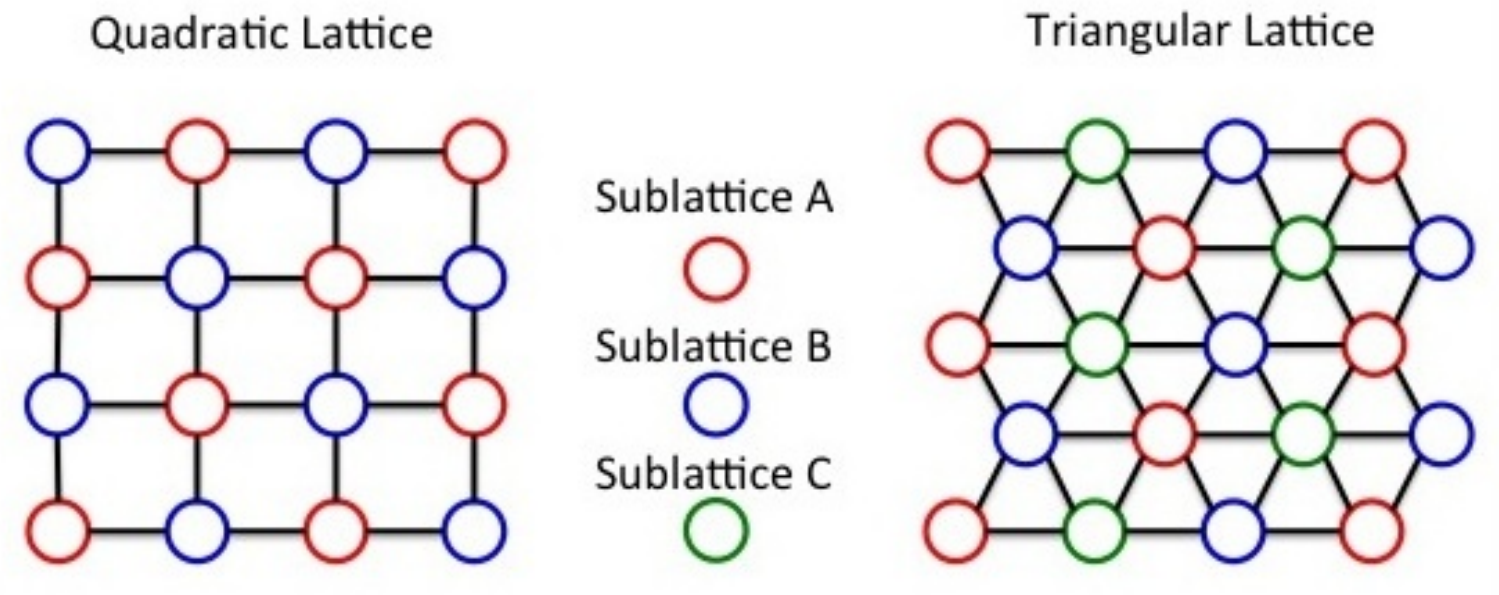
Hard-core limit:

$$a \to \infty \Rightarrow U \to \infty \Rightarrow n \in \{0, 1\}$$

Hamiltonian for hard-core bosons:

$$\hat{H} = -J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j + \frac{V}{2} \sum_{<i,j>} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i$$

# Patterns




not frustrated

frustrated

Connectivity matrices:

$$N = \begin{pmatrix} 0 & 4 \\ 4 & 0 \end{pmatrix}$$

$$N = \begin{pmatrix} 0 & 3 & 3 \\ 3 & 0 & 3 \\ 3 & 3 & 0 \end{pmatrix}$$

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# Mean-field approximation

Problem: bilocal terms in Hamiltonian

Mean-field approximation:

$$\hat{a}_i = \langle \hat{a}_i \rangle + \delta \hat{a}_i$$
$$\hat{a}_i^\dagger = \left\langle \hat{a}_i^\dagger \right\rangle + \delta \hat{a}_i^\dagger$$
$$\hat{n}_i = \langle \hat{n}_i \rangle + \delta \hat{n}_i$$

$$\delta \hat{a}_i^\dagger \delta \hat{a}_j \approx 0 \quad \forall i, j$$

$$\delta \hat{n}_i \delta \hat{n}_j \approx 0 \quad \forall i, j$$

Operators appearing in the Hamiltonian:

$$\begin{aligned} \hat{a}_i^\dagger \hat{a}_j &\approx \left\langle \hat{a}_i^\dagger \right\rangle \hat{a}_j + \langle \hat{a}_j \rangle \hat{a}_i^\dagger - \left\langle \hat{a}_i^\dagger \right\rangle \langle \hat{a}_j \rangle \\ &= \psi_i^* \hat{a}_j + \psi_j \hat{a}_i^\dagger - \psi_i^* \psi_j \end{aligned}$$

$$\psi_i := \langle \hat{a}_i \rangle$$

$$\varrho_i := \langle \hat{n}_i \rangle$$

$$\begin{aligned} \hat{n}_i \hat{n}_j &\approx \langle \hat{n}_i \rangle \hat{n}_j + \langle \hat{n}_j \rangle \hat{n}_i - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle \\ &= \varrho_i \hat{n}_j + \varrho_j \hat{n}_i - \varrho_i \varrho_j \end{aligned}$$

# Mean-field Hamiltonian

## Hamiltonian for the whole lattice

$$\hat{H} \overset{MF}{\approx} \sum_i \hat{h}_{MF,i}$$

$$\Psi_i := \sum_{j \in NN_i} \psi_j$$

$$R_i := \sum_{j \in NN_i} \varrho_j$$

$$\begin{aligned} \hat{h}_{MF,i} \quad := \quad & -J\left(\hat{a}_i \Psi_i^* + \hat{a}_i^\dagger \Psi_i - \psi_i^* \Psi_i\right) \\ & + \frac{V}{2}\left(2\hat{n}_i R_i - \varrho_i R_i\right) \\ & - \mu \hat{n}_i \end{aligned}$$

# Mean-field Hamiltonian

## Hamiltonian for periodic patterns

For periodic patterns:
Hamiltonian reduces to a **sum over** the **finite number** of sites in the unit cell (UC).

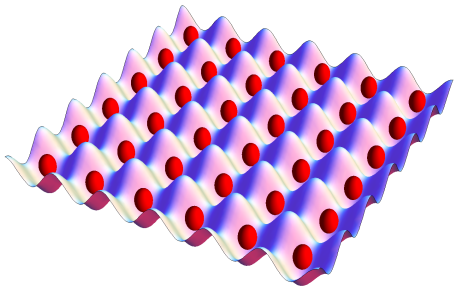
$$\hat{h}_{MF,UC} = \left(J\Psi - \frac{V}{2}R\right) - J\sum_X \left(\hat{a}_X\Psi_X^* + \hat{a}_X^\dagger\Psi_X\right) + 2\sum_X \hat{n}_X\left(\frac{V}{2}R_X - \frac{\mu}{2}\right)$$

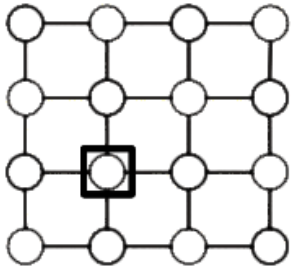
$$X \in \{A, B, \ldots\}, \qquad \Psi := \sum_X \psi_X^*\Psi_X, \qquad R := \sum_X \varrho_X R_X$$

# Usual calculation method

- Finding Hamiltonian for a special case (pattern)
- Defining a basis for the pattern
- Finding matrix representations for operators on this basis
  - For $n$ sites in the unit cell the **size of the matrix is** $2^n$**!**
- Combining them to the matrix representation of the Hamiltonian
- Solving the eigenvalue equation $\det\left(\hat{H} - E\right) = 0$
  - roots of $2^n$-**order polynomial !**
  - **no general solution** for the energies $E$ **to expect** !

# Homogeneous pattern



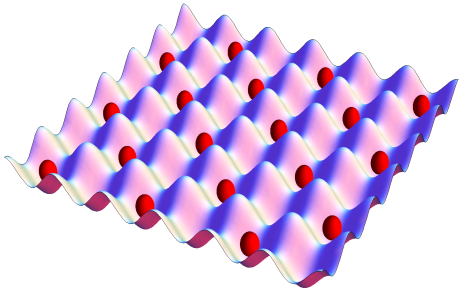


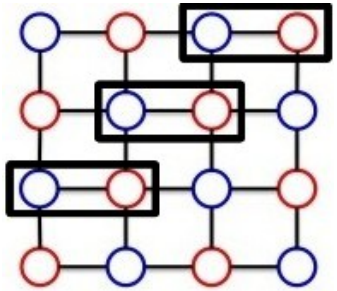
hard-core basis: $\mathcal{B} = \{|0\rangle, |1\rangle\}$

$$\left(\hat{h}_{MF,UC}\right)_{\mathcal{B}} = \begin{pmatrix} \left(J\Psi - \frac{V}{2}R\right) & -J\Psi_A^* \\ -J\Psi_A & \left(J\Psi - \frac{V}{2}R\right) + 2\left(\frac{V}{2}R_A - \frac{\mu}{2}\right) \end{pmatrix}$$

$$E_{\pm_A} = \left(J\Psi - \frac{V}{2}R\right) + \left(\frac{V}{2}R_A - \frac{\mu}{2}\right) \pm_A \sqrt{\left(\frac{V}{2}R_A - \frac{\mu}{2}\right)^2 + \left(J\left|\Psi_A\right|\right)^2}$$

# 2 sites in the unit cell





hard-core basis: $\mathcal{B} = \{|0,0\rangle, |1,0\rangle, |0,1\rangle, |1,1\rangle\}$

$$\begin{pmatrix} (J\Psi - \frac{V}{2}R) & -J\Psi_A^* & -J\Psi_B^* & \\ -J\Psi_A & (J\Psi - \frac{V}{2}R) + 2\left(\frac{V}{2}R_A - \frac{\mu}{2}\right) & & -J\Psi_B^* \\ -J\Psi_B & & (J\Psi - \frac{V}{2}R) + 2\left(\frac{V}{2}R_B - \frac{\mu}{2}\right) & -J\Psi_A^* \\ & -J\Psi_B & -J\Psi_A & (J\Psi - \frac{V}{2}R) + 2\left(\frac{V}{2}R_A - \frac{\mu}{2}\right) + 2\left(\frac{V}{2}R_B - \frac{\mu}{2}\right) \end{pmatrix}$$

$$\begin{aligned} E_{\pm_A,\pm_B} = & \left(J\Psi - \frac{V}{2}R\right) \\ & + \left(\frac{V}{2}R_A - \frac{\mu}{2}\right) \pm_A \sqrt{\left(\frac{V}{2}R_A - \frac{\mu}{2}\right)^2 + (J|\Psi_A|)^2} \\ & + \left(\frac{V}{2}R_B - \frac{\mu}{2}\right) \pm_B \sqrt{\left(\frac{V}{2}R_B - \frac{\mu}{2}\right)^2 + (J|\Psi_B|)^2} \end{aligned}$$

# Energies

## General formula for the energies

$$
\begin{aligned}
E_{\pm_{\boldsymbol{A}}} &= \left(J\Psi - \frac{V}{2}R\right) + \left(\frac{V}{2}R_{\boldsymbol{A}} - \frac{\mu}{2}\right) \pm_{\boldsymbol{A}} \sqrt{\left(\frac{V}{2}R_{\boldsymbol{A}} - \frac{\mu}{2}\right)^{2} + (J\,|\Psi_{\boldsymbol{A}}|)^{2}} \\
E_{\pm_{\boldsymbol{A}},\pm_{\boldsymbol{B}}} &= \left(J\Psi - \frac{V}{2}R\right) \\
&\quad + \left(\frac{V}{2}R_{\boldsymbol{A}} - \frac{\mu}{2}\right) \pm_{\boldsymbol{A}} \sqrt{\left(\frac{V}{2}R_{\boldsymbol{A}} - \frac{\mu}{2}\right)^{2} + (J\,|\Psi_{\boldsymbol{A}}|)^{2}} \\
&\quad + \left(\frac{V}{2}R_{\boldsymbol{B}} - \frac{\mu}{2}\right) \pm_{\boldsymbol{B}} \sqrt{\left(\frac{V}{2}R_{\boldsymbol{B}} - \frac{\mu}{2}\right)^{2} + (J\,|\Psi_{\boldsymbol{B}}|)^{2}}
\end{aligned}
$$

$$
\begin{aligned}
E_{\pm_{\boldsymbol{A}},\pm_{\boldsymbol{B}},\ldots} &= \left(J\Psi - \frac{V}{2}R\right) \\
&\quad + \sum_{\boldsymbol{X}} \left(\frac{V}{2}R_{\boldsymbol{X}} - \frac{\mu}{2}\right) \\
&\quad + \sum_{\boldsymbol{X}} (\pm_{\boldsymbol{X}}) \sqrt{\left(\frac{V}{2}R_{\boldsymbol{X}} - \frac{\mu}{2}\right)^{2} + (J\,|\Psi_{\boldsymbol{X}}|)^{2}}
\end{aligned}
$$

# Finding the mean-field parameters

$$\partial_{\varrho_X} E = 0 \quad \forall X, \qquad\qquad \partial_{\psi_X} E = 0 \quad \forall X$$

leading to:

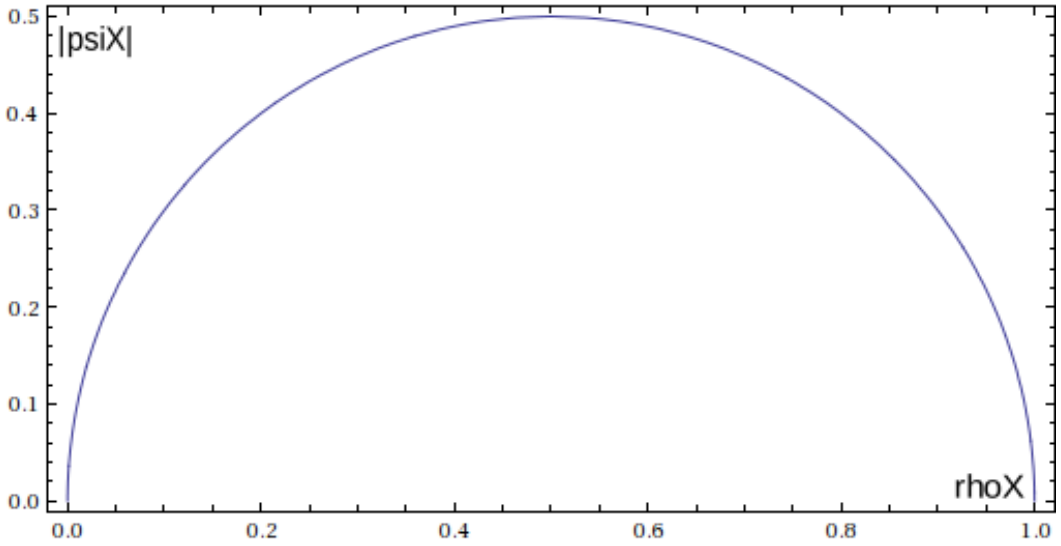
$$\left(\varrho_X - \tfrac{1}{2}\right) = \tfrac{1}{2}\left(\pm_X\right) \frac{\left(\frac{V}{2} R_X - \frac{\mu}{2}\right)}{\sqrt{\left(\frac{V}{2} R_X - \frac{\mu}{2}\right)^2 + (J|\Psi_X|)^2}},$$

$$\psi_X = -\tfrac{1}{2}\left(\pm_X\right) \frac{J\Psi_X}{\sqrt{\left(\frac{V}{2} R_X - \frac{\mu}{2}\right)^2 + (J|\Psi_X|)^2}}$$

# Resulting formulas

## Relation between $\varrho$ and $\psi$ independent of other sites

$$\left(\varrho_X - \tfrac{1}{2}\right)^2 + |\psi_X|^2 = \tfrac{1}{4}$$




$$|\psi_X| = 0 \quad \Rightarrow \varrho_X \in \{0, 1\}$$

no hopping $\Rightarrow$ bosons localized in valleys

$\Rightarrow$ expectation value for density: 0 (absent) or 1 (present)

# Resulting formulas

## Relation between $\varrho$'s and $\psi$'s of different sites

$$\eta_{\boldsymbol{X}} \quad \underset{\Downarrow}{:=} \quad \frac{\Psi_{\boldsymbol{X}}}{\psi_{\boldsymbol{X}}}$$

$$\underbrace{\begin{pmatrix} N_{X_1,X_1} & N_{X_1,X_2} & \cdots \\ N_{X_2,X_1} & N_{X_2,X_2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}_{\text{reduced connectivity matrix}} \begin{pmatrix} \psi_{X_1} \\ \psi_{X_2} \\ \vdots \end{pmatrix} = \begin{pmatrix} \eta_{X_1} & 0 & \cdots \\ 0 & \eta_{X_2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \psi_{X_1} \\ \psi_{X_2} \\ \vdots \end{pmatrix}$$

$$\begin{pmatrix} \varrho_{X_1} \\ \varrho_{X_2} \\ \vdots \end{pmatrix} = \left( J \begin{pmatrix} \eta_{X_1} & 0 & \cdots \\ 0 & \eta_{X_2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} + \frac{V}{2} \overbrace{\begin{pmatrix} N_{X_1,X_1} & N_{X_1,X_2} & \cdots \\ N_{X_2,X_1} & N_{X_2,X_2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}^{\text{reduced connectivity matrix}} \right)^{-1}$$

$$\times \begin{pmatrix} \frac{1}{2} J \eta_{X_1} + \frac{\mu}{2} - \frac{V}{2} \sum_j N_{Y_j X_1} \, (01)_{Y_j} \\ \frac{1}{2} J \eta_{X_2} + \frac{\mu}{2} - \frac{V}{2} \sum_j N_{Y_j X_2} \, (01)_{Y_j} \\ \vdots \end{pmatrix}$$

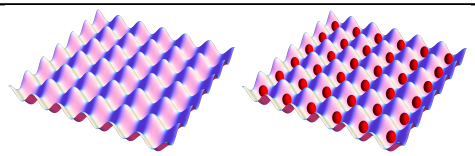
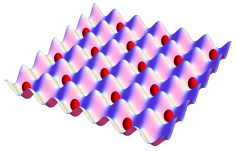
$X_i \in \mathbb{M}_{\psi \neq 0} \forall i$ $\qquad$ $Y_j \in \mathbb{M}_{\psi = 0} \forall j$ $\qquad$ $\varrho_{Y_j} = (01)_{Y_j} \in \{0, 1\}$

# Resulting formulas

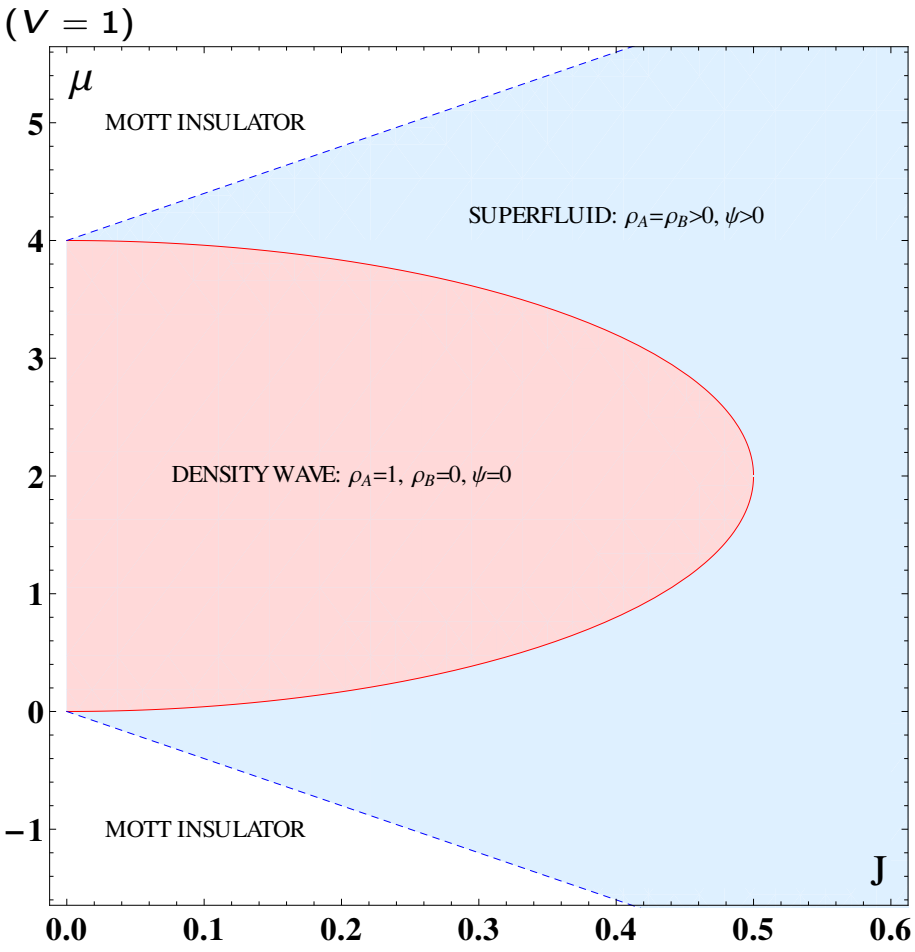
## Energies

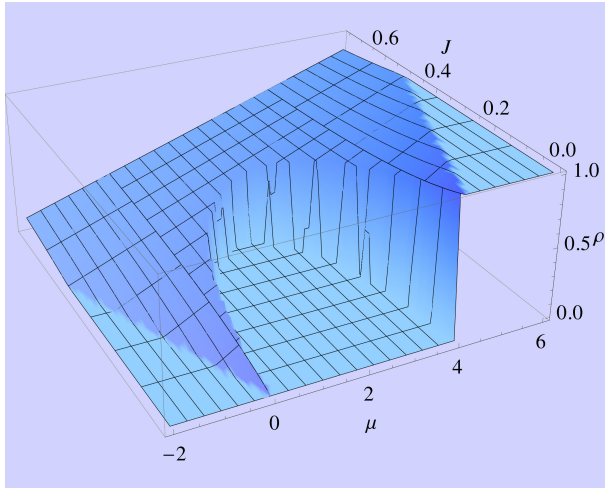
$$
\begin{aligned}
&\frac{E\left(\varrho_{\boldsymbol{A}}\left(\frac{\boldsymbol{J}}{\boldsymbol{V}},\frac{\mu}{\boldsymbol{V}}\right),\varrho_{\boldsymbol{B}}\left(\frac{\boldsymbol{J}}{\boldsymbol{V}},\frac{\mu}{\boldsymbol{V}}\right),\ldots,\eta_{\boldsymbol{A}},\eta_{\boldsymbol{B}},\ldots\right)}{V} \\
= \quad & \underbrace{\frac{1}{2}\sum_{\boldsymbol{X}\in\mathbb{M}_{\psi=\boldsymbol{0}}}\sum_{\boldsymbol{Y}\in\mathbb{M}_{\psi=\boldsymbol{0}}} N_{\boldsymbol{XY}}\varrho_{\boldsymbol{Y}}\varrho_{\boldsymbol{X}} - \frac{\mu}{V}\sum_{\boldsymbol{X}\in\mathbb{M}_{\psi=\boldsymbol{0}}}\varrho_{\boldsymbol{X}}}_{=:\frac{\boldsymbol{E}_{\psi=\boldsymbol{0}}}{\boldsymbol{V}}} \\
& \underbrace{+\frac{1}{2}\sum_{\boldsymbol{X}\in\mathbb{M}_{\psi=\boldsymbol{0}}}\sum_{\boldsymbol{Y}\in\mathbb{M}_{\psi\neq\boldsymbol{0}}} N_{\boldsymbol{XY}}\varrho_{\boldsymbol{Y}}\varrho_{\boldsymbol{X}}}_{=:\frac{\boldsymbol{E}_{\boldsymbol{mix}}}{\boldsymbol{V}}} \\
& \underbrace{-\frac{1}{2}\sum_{\boldsymbol{X}\in\mathbb{M}_{\psi\neq\boldsymbol{0}}}\varrho_{\boldsymbol{X}}\left(\frac{J}{V}\eta_{\boldsymbol{X}}+\frac{\mu}{V}\right)}_{=:\frac{\boldsymbol{E}_{\psi\neq\boldsymbol{0}}}{\boldsymbol{V}}}
\end{aligned}
$$

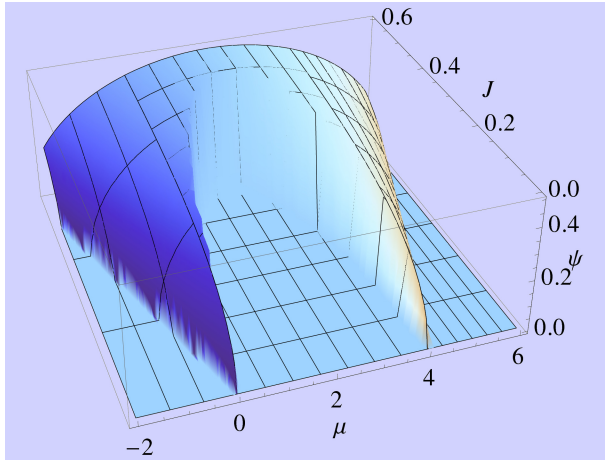
# Possible phases

| | $\varrho$ | $\psi$ | |
|---|---|---|---|
| Mott | $\forall \boldsymbol{X}, \boldsymbol{Y} \quad \varrho_{\boldsymbol{X}} = \varrho_{\boldsymbol{Y}}$ | $\forall \boldsymbol{X} \quad \psi_{\boldsymbol{X}} = 0$ |  |
| Density wave | $\exists \boldsymbol{X}, \boldsymbol{Y} \quad \varrho_{\boldsymbol{X}} \neq \varrho_{\boldsymbol{Y}}$ | $\forall \boldsymbol{X} \quad \psi_{\boldsymbol{X}} = 0$ |  |
| Superfluid | $\forall \boldsymbol{X}, \boldsymbol{Y} \quad \varrho_{\boldsymbol{X}} = \varrho_{\boldsymbol{Y}}$ | $\forall \boldsymbol{X}, \boldsymbol{Y} \quad \psi_{\boldsymbol{X}} = \psi_{\boldsymbol{Y}} \neq 0$ | |
| Supersolid | $\exists \boldsymbol{X}, \boldsymbol{Y} \quad \varrho_{\boldsymbol{X}} \neq \varrho_{\boldsymbol{Y}}$ | $\exists \boldsymbol{X}, \boldsymbol{Y} \quad \psi_{\boldsymbol{X}} \neq \psi_{\boldsymbol{Y}} \neq 0$ | |

# Quadratic lattice

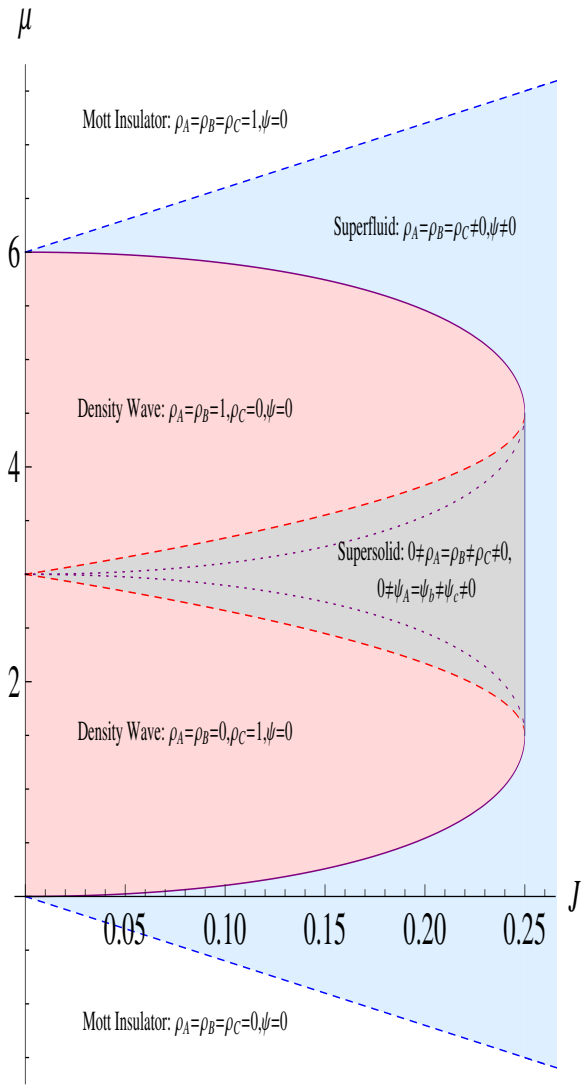


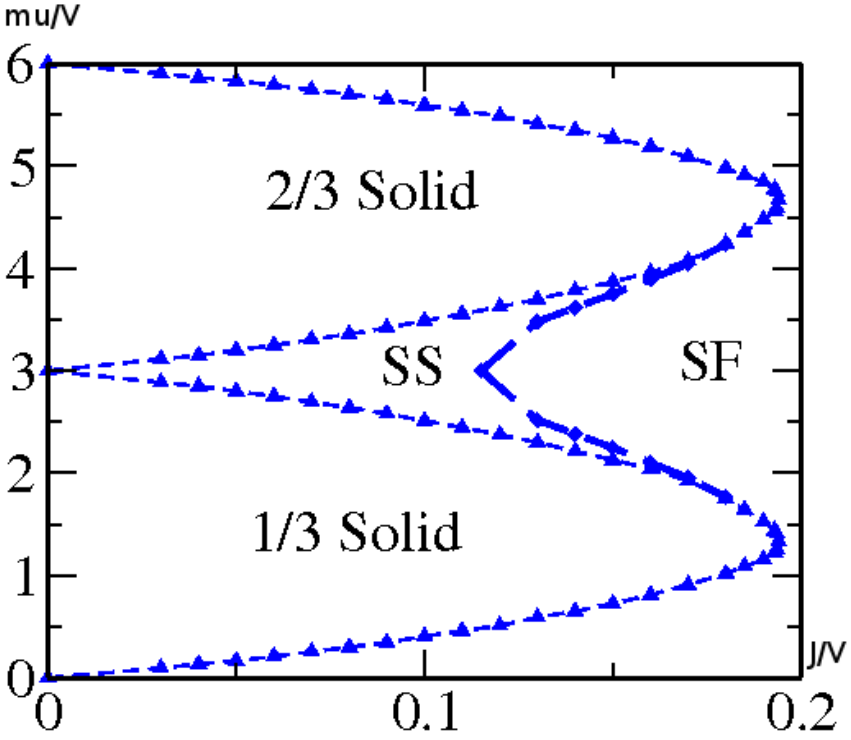



# Triangular lattice

$(V = 1)$




X.-F. Zhang, R. Dillenschneider, Y. Yu and S. Eggert, Phys. Rev. B 84, 174515 (2011)

G. Murthy, D. Arovas, A. Auerbach, Phys. Rev. B 55, 3104 (1996)

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# Negative hopping $J$

## Quadratic lattice

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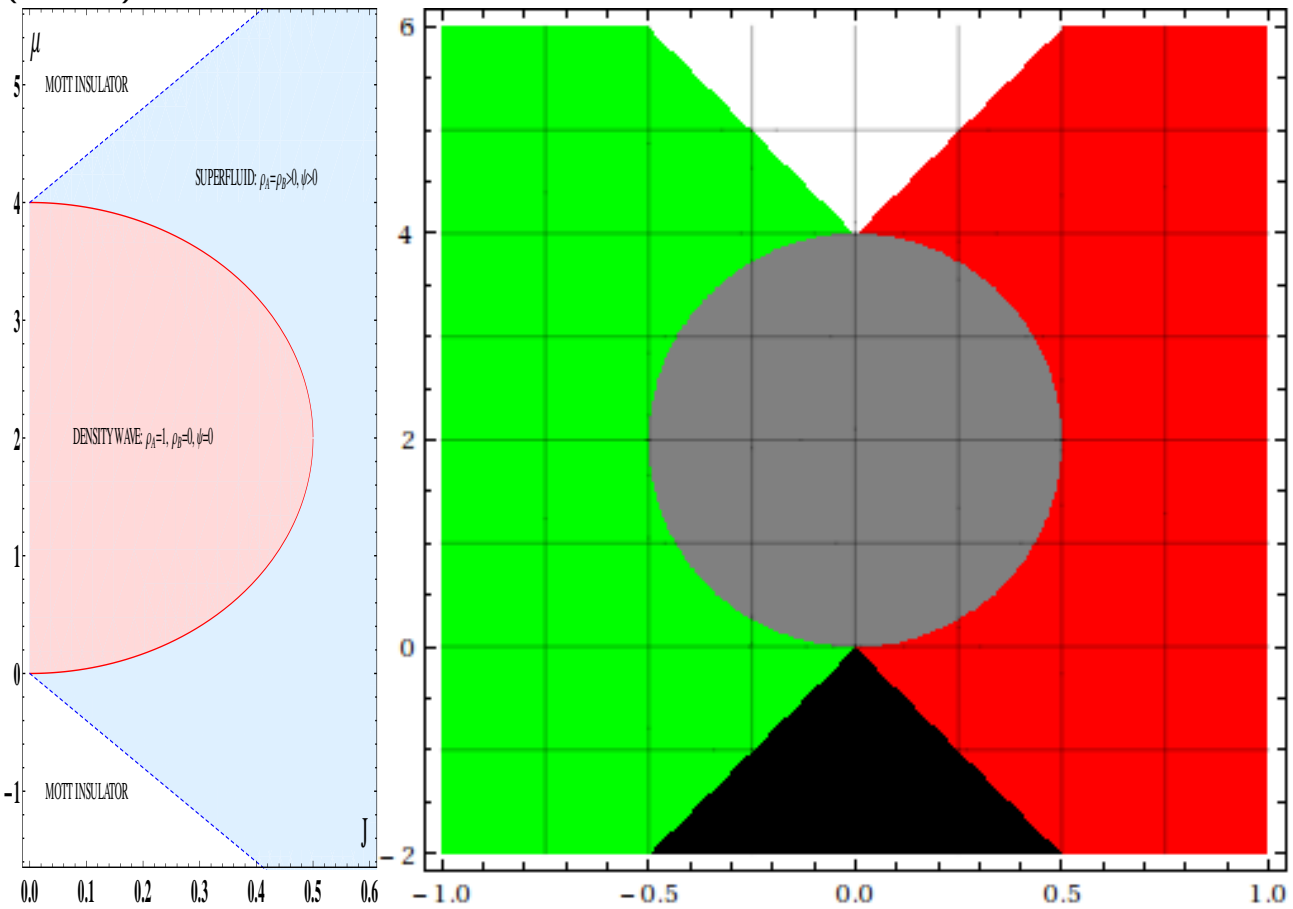


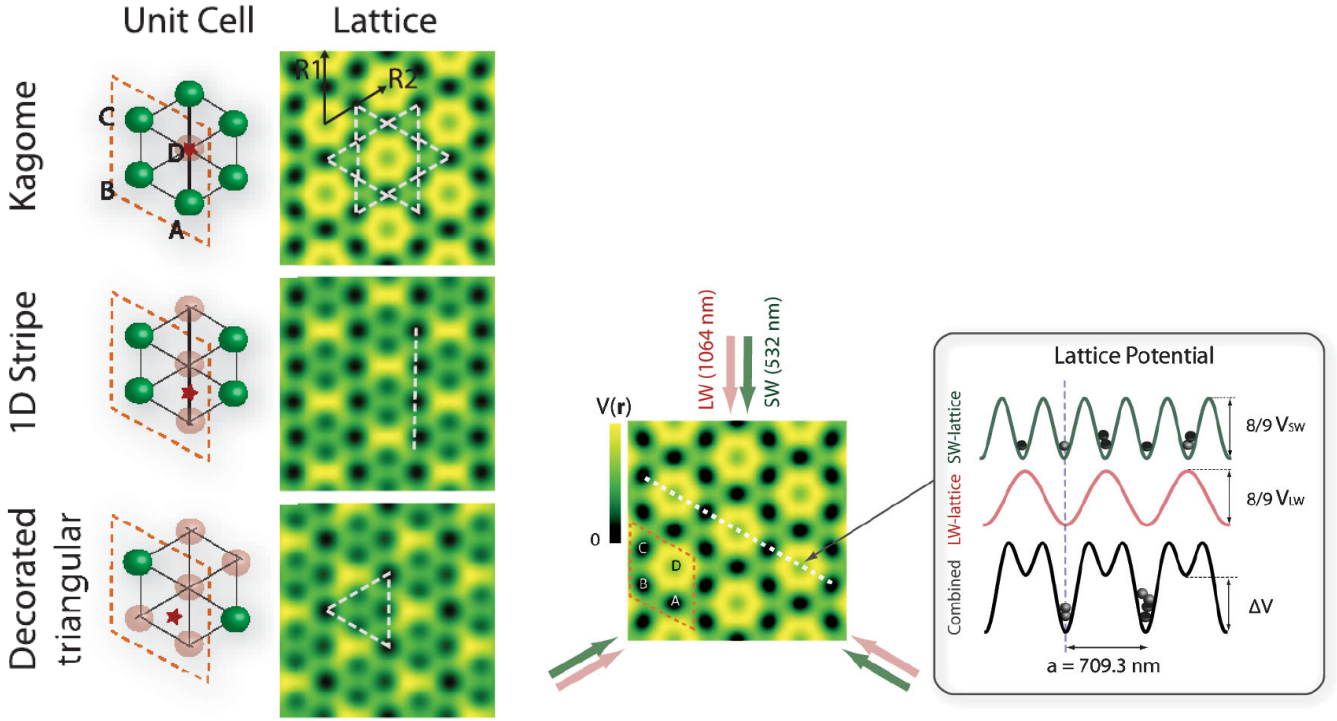

SF1:
$|\psi_A| = |\psi_B|$
$\mathrm{sign}\psi_A = \mathrm{sign}\psi_B$

SF2:
$|\psi_A| = |\psi_B|$
$\mathrm{sign}\psi_A = -\mathrm{sign}\psi_B$


A. Eckardt, C. Weiss, and M. Holthaus, Phys. Rev. Lett., 95, 260404 (2005)
A. Zenesini, H.Lignier, C. Sias, O. Morsch, D. Ciampini, E. Arimondo, Phys. Rev. Lett., 102, 100403 (2009)

# Other lattices

## Kagome, 1D Stripe, decorated triangular, ...




G.-B. Jo, J. Guzman, C. K. Thomas, P. Hosur, A. Vishwanath and D. M. Stamper-Kurn, PRL 108, 045305 (2012)

# Quantum corrections

inspired by variational perturbation theory
(H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, World Scientific Publishing Company, 5th edition (2009))

$$\hat{H}(\xi) = \hat{H}_{MF} + \xi\left(\hat{H}_{BH} - \hat{H}_{MF}\right)$$

- Free energy:
  $F(\xi) = -\frac{1}{\beta}\ln Z(\xi), \qquad Z(\xi) = \mathrm{Tr}\left(e^{-\beta\hat{H}(\xi)}\right)$
- Expansion with respect to $\xi$:
  $F(\xi) = F_{MF} + \xi\left\langle\hat{H} - \hat{H}_{MF}\right\rangle_{MF} + \ldots, \qquad \left\langle\hat{\mathcal{O}}\right\rangle_{MF} := \frac{1}{Z_{MF}}\mathrm{Tr}\left(\hat{\mathcal{O}}e^{-\beta\hat{H}_{MF}}\right)$
- Truncation after n-th order depends artificially on $\varrho_X$, $\psi_X$ for $\xi = 1$:
  $F^{(n)}(\xi = 1) = F^{(n)}(\varrho_X, \psi_X)$
- Principle of minimal sensitivity:
  $\partial_{\varrho_X} F^{(n)} = 0$, $\partial_{\psi_X} F^{(n)} = 0$
- Quantum corrections:

  $n = 0$: mean-field

  $n = 1$: first quantum corrections

  $n = 2$: ...

F. E. A. dos Santos and A. Pelster, Phys. Rev. A **79**, 013614 (2009)